Supporting Information

I_2-Catalyzed Oxidative C(sp^3)-H/S-H Coupling: Utilizing Un-activated Alkanes and Mercaptans as the Nucleophiles

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Table of Contents

General information

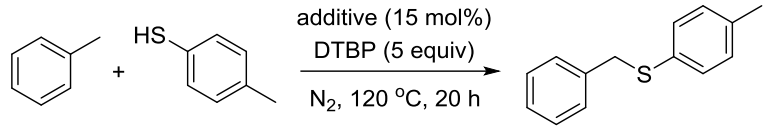
The reactions were conducted in Schlenk tube under N_2 atmosphere. All glassware was oven dried at 110 ℃ for 30 minutes and cooled down under vacuum. Unless otherwise noted, materials were obtained from commercial suppliers and used without further purification. Thin layer chromatography (TLC) employed glass 0.25 mm silica gel plates. Flash chromatography columns were packed with 200-300 mesh silica gel in petroleum (bp. 60-90 ℃). GC-MS spectra were recorded on a Varian GC-MS 3900-2100T. EPR spectra were recorded on a Bruker A-200 spectrometer. For the *in situ* IR experiments, the reaction spectra were recorded using an iC 15 from Mettler-Toledo AutoChem, Inc. Data manipulation was carried out using the iC IR software (Ver. 4.3.27, Mettler-Toledo AutoChem, Inc.). ^{1}H and ^{13}C NMR data were recorded with Bruker ADVANCE III (400 MHz) spectrometers with tetramethylsilane as an internal standard. All chemical shifts (δ) are reported in ppm and coupling constants (*J*) in Hz. All chemical shifts are reported relative to tetramethylsilane and d-solvent peaks (77.3 ppm, chloroform), respectively. High resolution mass spectra (HRMS) were measured with a Waters Micromass GCT instrument, accurate masses are reported for the molecular ion ($[M]^+$).

General procedure of the oxidative C(sp^3)-H/S-H bond formation

To a Schlenk tube charged with I_2 (0.045 mmol) was added alkane (4.0 mL) under N_2 atmosphere. After the dissolution of the I_2, mercaptan (0.3 mmol) was added followed by the injection of DTBP (1.5 mmol) via a microsyringe. Then the Schlenk tube was allowed to be heated to 120 ºC for 20 h. After the completion of the reaction, it was quenched by water (5 mL) and extracted with ethyl acetate (3 × 4 mL). The organic layers were combined and evaporated under vacuum. The pure product was obtained by flash chromatography on silicagel using petroleum ether and dichloromethane/ethyl acetate as the eluent.

Condition Optimization of the oxidative C(sp^3)-H/S-H bond formation

Table S1. Condition optimization of the oxidative C(sp^3)-H/S-H bond formation



1a **2a** **3aa**

entry	additive	oxidant	GC yield [%][b]
1	I_2	DDQ	n. d.
2	I_2	$K_2S_2O_8$	n. d.
3	I_2	$PhI(OAc)_2$	n. d.
4	I_2	$(NH_4)_2Ce(NO_3)_6$	n. d.
5	I_2	H_2O_2	n. d.
6	I_2	DTBP	74
7	$^nBu_4NI$	DTBP	27
8	KI	DTBP	60
9	NIS	DTBP	67

Reaction conditions: **1a** (4 mL), **2a** (0.3 mmol), oxidant (1.5 mmol), additive (0.045 mmol) at 120 °C for 20 h under N_2. The yield was determined by GC analysis with biphenyl as the internal standard. n.d.= no desired product.

Procedure of the sampling reactions

GC-analyzed sampling reaction under standard condition: To a Schlenk tube charged with biphenyl (20 – 30 mg), I_2 (0.045 mmol) was added toluene (4.0 mL) under N_2 atmosphere. After the dissolution of the I_2, 4-methyl-thiophenyl (0.3 mmol) was added followed by the injection of DTBP (1.5 mmol) via a microsyringe. Then the Schlenk tube was allowed to be heated to 120 ^oC. 0.2 mL of the solution was taken out every hour through a long syringe needle until the end of the seventh hour. The taken out solution was analyzed by GC. Then the system was allowed to react for 13 hours and then analyzed by GC.

GC-analyzed sampling reaction under standard condition without I_2: To a Schlenk tube charged with biphenyl (20 – 30 mg) was added toluene (4.0 mL) under N_2 atmosphere. 4-methyl-thiophenyl (0.3 mmol) was then added followed by the injection of DTBP (1.5 mmol) via a microsyringe. Then the Schlenk tube was allowed to be heated to 120 ^oC. 0.2 mL of the solution was taken out every hour through a long syringe needle until the end of the seventh hour. The taken out solution was analyzed by GC. Then the system was allowed to react for 13 hours and then analyzed by GC.

Procedure of *in situ* IR experiment

To a three-neck vessel charged with I_2 (0.045 mmol) was added alkane (4.0 mL) under N_2 atmosphere. After the dissolution of the I_2, mercaptan (0.3 mmol) was added. Then the vessel was allowed to be heated to 120 °C. After that, DTBP (1.5 mmol) was injected via a microsyringe ant the system was monitored by *in situ* IR for 20 minutes. Then the reaction was quenched by water (5 mL) and then analyzed by GC.

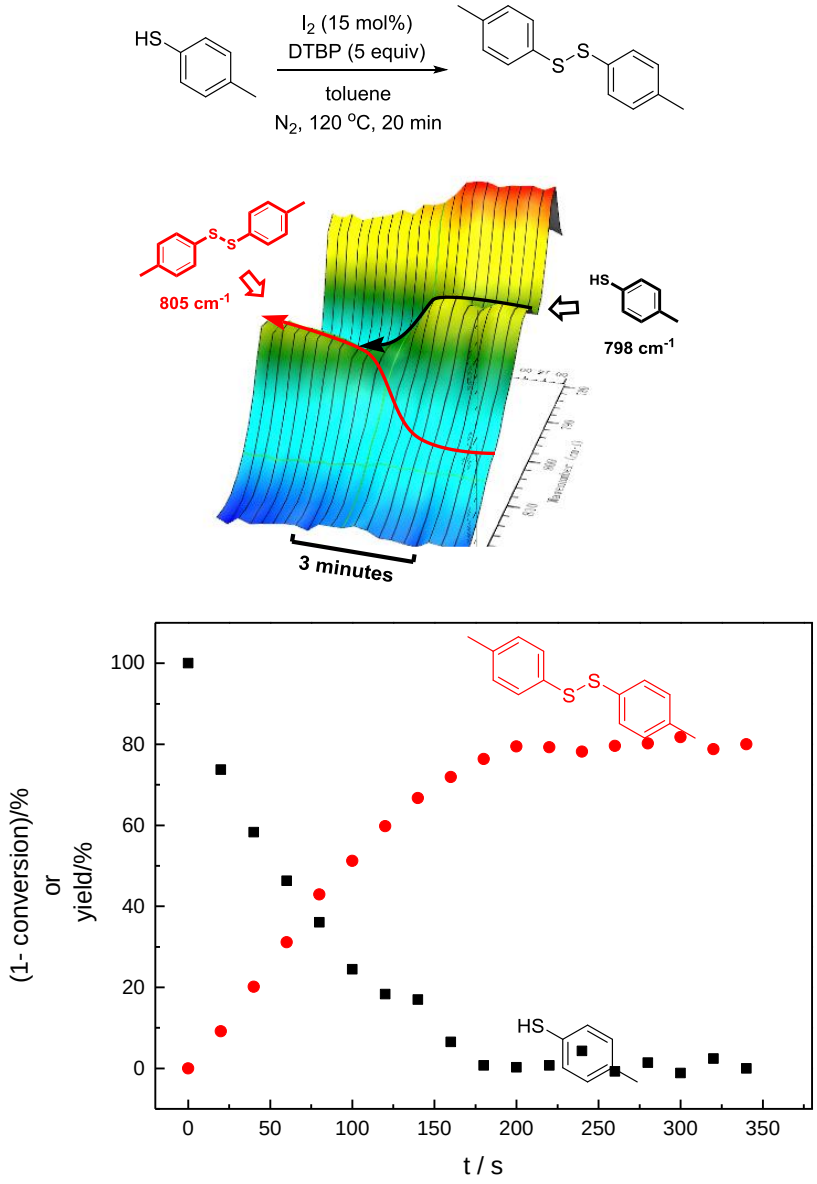


Figure S1. *In situ* IR result of the dimerization of mercaptans.

Procedure of the EPR experiment

To a Schlenk tube (charged with I_2 or both I_2 and 4-methylphenyl disulfide if necessary) was added toluene or cyclohexane (2.0 mL) under N_2 atmosphere, then DTBP (1.5 mmol) was injected via a microsyringe. After that, the Schlenk tube was allowed to be heated to 120 ºC for 5 h. 10 μL DMPO (5-,5-dimethyl-1-pyrroline N-oxide) was added before 10 μL of the solution was taken out into a small tube. Then, this mixture was analyzed by EPR at room temperature.

Procedure of the control experiments and radical trapping experiment

Blank experiment: To a Schlenk tube was added toluene (4.0 mL) under N_2 atmosphere. 4-methoxy-thiophenyl (0.3 mmol) was added followed by the injection of DTBP (1.5 mmol) via a microsyringe. Then the Schlenk tube was allowed to be heated to 120 ^oC for 20 h. Then the reaction was analyzed by GC.

Disulfide as substrate: To a Schlenk tube charged with I_2 (0.045 mmol) was added toluene (4.0 mL) under N_2 atmosphere. 4-methoxy-phenyl disulfide (0.15 mmol) was added followed by the injection of DTBP (1.5 mmol) via a microsyringe. Then the Schlenk tube was allowed to be heated to 120 ^oC for 20 h. Then the reaction was analyzed by GC.

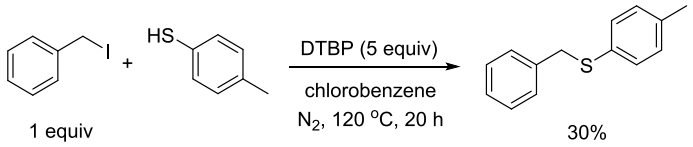
Radical trapping experiment: To a Schlenk tube charged with BHT (0.3 mmol), I_2 (0.045 mmol) was added toluene (4.0 mL) under N_2 atmosphere. After the dissolution of the I_2, 4-methoxy-thiophenyl (0.3 mmol) was added followed by the injection of DTBP (1.5 mmol) via a microsyringe. Then the Schlenk tube was allowed to be heated to 120 ^oC for 20 h. Then the reaction was analyzed by GC.

Procedure of the KIE experiment

To a Schlenk tube charged with I_2 (0.045 mmol) was added toluene (2.0 mL) and toluene-d_8 (2.0 mL) under N_2 atmosphere. After the dissolution of the I_2, 4-methoxy-thiophenyl (0.3 mmol) was added followed by the injection of DTBP (1.5 mmol) via a microsyringe. Then the Schlenk tube was allowed to be heated to 120 ^oC for 20 h. After the completion of the reaction, it was quenched by water (5 mL) and extracted with ethyl acetate (3 × 4 mL). The organic layers were combined and evaporated under vacuum. The pure product was obtained by flash chromatography on silica gel using petroleum ether and dichloromethane as the eluent. The value of k_H/k_D was determined by ^1H NMR.

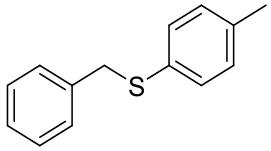
Procedure of the substitution of benzyl iodide

To a Schlenk tube charged with benzyl iodide (0.3 mmol) was added chlorobenzene (4.0 mL) under N_2 atmosphere. 4-mehtyl-thiophenyl (0.3 mmol) was added followed by the injection of DTBP (1.5 mmol) via a microsyringe. Then the Schlenk tube was allowed to be heated to 120 ^oC for 20 h. Then the reaction was analyzed by GC.

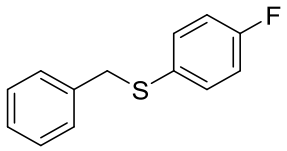


Scheme S1. Substitution of benzyl iodide.

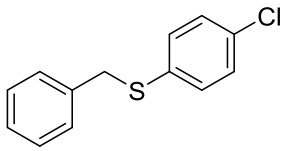
Detailed descriptions for products



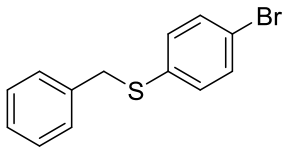
Benzyl phenyl sulfide (3aa)[1]: white solid was obtained with 74% yield. Eluent: Petroleum ether: CH_2Cl_2 = 200:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.36 – 7.24 (m, 7H), 7.11 (d, *J* = 7.6, 2H), 4.12 (s, 2H), 2.36 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 137.8, 136.6, 132.5, 130.7, 129.6, 128.9, 128.5, 127.1, 39.8, 21.1.



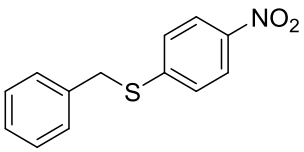
Benzyl 4-fluorophenyl sulfide (3ab)[2]: colorless liquid was obtained with 73% yield. Eluent: Petroleum ether: CH_2Cl_2 = 200:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.37 – 7.22 (m, 7H), 7.03 – 6.95 (m, 2H), 4.13 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.1 (d, *J* = 246.8 Hz), 137.5 , 133.4 (d, *J* = 8.1 Hz), 130.7 (d, *J* = 3.5 Hz), 128.9 , 128.5 , 127.2 , 115.9 (d, *J* = 21.7 Hz), 40.5.



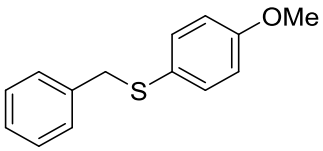
Benzyl 4-chlorophenyl sulfide (3ac)[3]: white solid was obtained with 77% yield. Eluent: Petroleum ether: CH_2Cl_2 = 200:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.39 – 7.27 (m, 5H), 7.26 (s, 4H), 4.13 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 137.1, 134.7, 132.5, 131.4, 129.0, 128.8, 128.6, 127.4, 39.3.



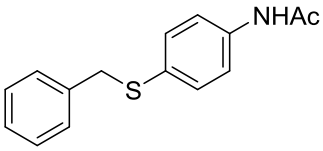
Benzyl 4-bromophenyl sulfide (3ad)[4]: white solid was obtained with 69% yield. Eluent: Petroleum ether: CH_2Cl_2 = 200:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.43 – 7.38 (m, 2H), 7.37 – 7.27 (m, 5H), 7.23 – 7.16 (m, 2H), 4.12 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 137.0, 135.4, 131.9, 131.4, 128.8, 128.6, 127.4, 120.3, 39.1.



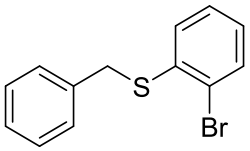
Benzyl 4-methoxyphenyl sulfide (3ae)[1]: light yellow solid was obtained with 40% yield. Eluent: Petroleum ether: CH_2Cl_2 = 5:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.13 (d, *J*=8.9, 2H), 7.48 – 7.30 (m, 7H), 4.28 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 147.3, 145.2, 135.4, 128.9, 128.7, 127.8, 126.6, 124.0, 37.0.



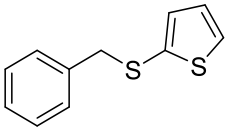
Benzyl 4-nitrophenyl sulfide (3af)[3]: colorless liquid was obtained with 86% yield. Eluent: Petroleum ether: CH_2Cl_2 = 10:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 – 7.22 (m, 7H), 6.85 (d, *J* = 8.8 Hz, 2H), 4.04 (s, 2H), 3.82 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 159.2, 138.2, 134.1, 128.9, 128.4, 127.0, 126.1, 114.5, 55.3, 41.3.



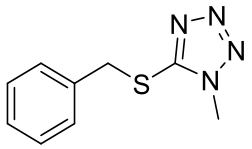
Benzyl 4-nitrophenyl sulfide (3ag): white solid was obtained with 60% yield. Eluent: Petroleum ether: ethyl acetate = 1:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 – 7.69 (b, 1H), 7.43 (d, *J* = 8.3 Hz, 2H), 7.36 – 7.20 (m, 7H), 4.08 (s, 2H), 2.18 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 168.7, 137.6, 136.8, 131.7, 131.0, 128.9, 128.5, 127.2, 120.3, 40.0, 24.6. HRMS (EI) calcd for $C_{15}H_{15}NOS$ $[M]^+$: 257.0874; found: 257.0871.



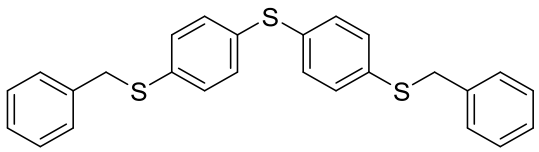
Benzyl 2-brmophenyl sulfide (3ah)[4]: colorless liquid was obtained with 74% yield. Eluent: Petroleum ether: CH_2Cl_2 = 200:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.63 – 7.57 (m, 1H), 7.45 – 7.40 (m, 2H), 7.40 – 7.24 (m, 5H), 7.10 – 7.04 (m, 1H), 4.20 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 138.0, 136.1, 133.0, 129.0, 128.7, 128.7, 127.8, 127.5, 126.9, 123.6, 37.9.



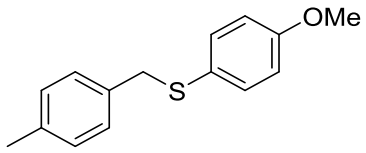
Benzyl 2-thienyl sulfide (3ai): colorless liquid was obtained with 70% yield. Eluent: Petroleum ether: CH_2Cl_2 = 200:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.42 – 7.30 (m, 4H), 7.30 – 7.22 (m, 1H), 7.13 – 6.95 (m, 2H), 4.05 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) ^{13}C NMR (101 MHz, $CDCl_3$) δ = 137.7, 134.5, 133.6, 129.9, 129.1, 128.5, 127.6, 127.3, 43.9. HRMS (EI) calcd for $C_{11}H_{10}S_2$ $[M]^+$: 206.0224; found: 206.0223.



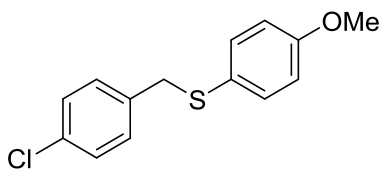
5-(Benzylthio)-1-methyl-tetrazole (3aj): colorless liquid was obtained with 38% yield. Eluent: Petroleum ether: ethyl acetate = 5:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.45 – 7.30 (m, 5H), 4.54 (s, 2H), 3.81 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 153.6, 135.6, 129.1, 128.9, 128.2, 37.9, 33.4. HRMS (EI) calcd for $C_9H_{10}N_4S$ $[M]^+$: 206.0626; found: 206.0624.



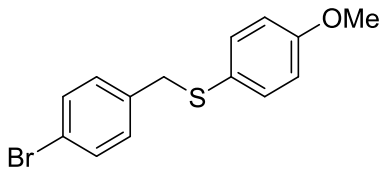
Bis(4-(benzylthio)phenyl)sulfide (3ak): white solid was obtained with 72% yield. Eluent: Petroleum ether: CH_2Cl_2 = 200:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.36 – 7.20 (m, 18H), 4.14 (s, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 137.1, 135.7, 133.5, 131.3, 130.3, 128.8, 128.6, 127.3, 38.9. HRMS (EI) calcd for $C_{26}H_1N_4S$ $[M]^+$: 430.0884; found: 430.0887.



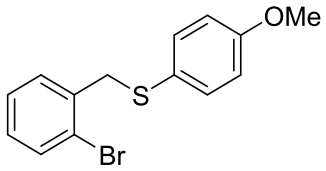
4-Methylbenzyl 4-methoxyphenyl sulfide (3bf): colorless liquid was obtained with 78% yield. Eluent: Petroleum ether: CH_2Cl_2 = 10:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.39 – 7.32 (m, 2H), 7.23 – 7.12 (m, 4H), 6.92 – 6.82 (m, 2H), 4.05 (s, 2H), 3.83 (s, 3H), 2.40 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 159.1, 136.6, 135.0, 133.9, 129.1, 128.8, 126.4, 114.4, 55.3, 40.9, 21.2. HRMS (EI) calcd for $C_{15}H_{16}OS$ $[M]^+$: 244.0922; found: 244.0921.



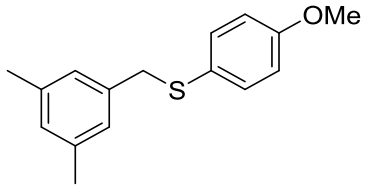
4-Chlorobenzyl 4-methoxyphenyl sulfide (3cf): colorless liquid was obtained with 68% yield. Eluent: Petroleum ether: CH_2Cl_2 = 10:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ7.28 – 7.22 (m, 4H), 7.11 (d, *J* = 8.4 Hz, 2H), 6.82 (d, *J* = 8.8 Hz, 2H), 3.95 (s, 2H), 3.81 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.4, 136.8, 134.5, 132.7, 130.2, 128.5, 125.3, 114.5, 55.3, 40.6. HRMS (EI) calcd for $C_{14}H_{13}ClOS$ $[M]^+$: 264.0376; found: 264.0371



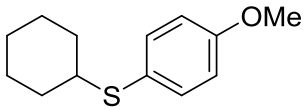
4-Bromobenzyl 4-methoxyphenyl sulfide (3df)[2]: white solid was obtained with 66% yield. Eluent: Petroleum ether: CH_2Cl_2 = 10:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.39 (d, *J* = 8.4, 2H), 7.26 (d, *J* = 8.7, 2H), 7.06 (d, *J* = 8.3, 2H), 6.82 (d, *J*=8.7, 2H), 3.93 (s, 2H), 3.81 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 159.4, 137.3, 134.5, 131.4, 130.6, 125.3, 120.8, 114.5, 55.3, 40.7.



2-Bromobenzyl 4-methoxyphenyl sulfide (3ef): colorless liquid was obtained with 70% yield. Eluent: Petroleum ether: CH_2Cl_2 = 10:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.58 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.33 – 7.28 (m, 2H), 7.21 – 7.06 (m, 3H), 6.95 – 6.66 (m, 2H), 4.12 (s, 2H), 3.82 (s, 3H). ^{13}C NMR (101 MHz, CDCl3) δ = 159.5, 137.4, 134.9, 133.0, 130.9, 128.7, 127.2, 125.4, 124.5, 114.5, 55.3, 41.8. HRMS (EI) calcd for $C_{14}H_{13}BrOS$ $[M]^+$: 307.9870; found: 307.9874.

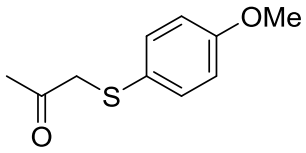


3,5-Dimethylbenzyl 4-methoxyphenyl sulfide (3ff): colorless liquid was obtained with 79% yield. Eluent: Petroleum ether: CH_2Cl_2 = 10:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.40 – 7.30 (m, 2H), 6.96 – 6.84 (m, 5H), 4.00 (s, 2H), 3.84 (s, 3H), 2.33 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 159.1, 137.9, 137.7, 133.8, 128.8, 126.8, 126.6, 114.4, 55.4, 41.2, 21.3. HRMS (EI) calcd for $C_{16}H_{18}OS$ $[M]^+$: 258.1078; found: 258.1074.

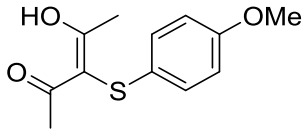


Cyclohexyl 4-methoxyphenyl sulfide (5af)[5]: colorless liquid was obtained with 80% yield. Eluent: Petroleum ether: CH_2Cl_2 = 10:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.42 (d, *J*=8.8, 2H), 6.87 (d, *J*=8.8, 2H), 3.83 (s, 3H), 2.99 – 2.88 (m, 1H), 2.00 – 1.92 (m, 2H), 1.83 – 1.73 (m, 2H), 1.66 – 1.58 (m,

1H), 1.40 – 1.21 (m, 5H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 159.3, 135.6, 124.9, 114.3, 55.3, 47.9, 33.4, 26.1, 25.8.



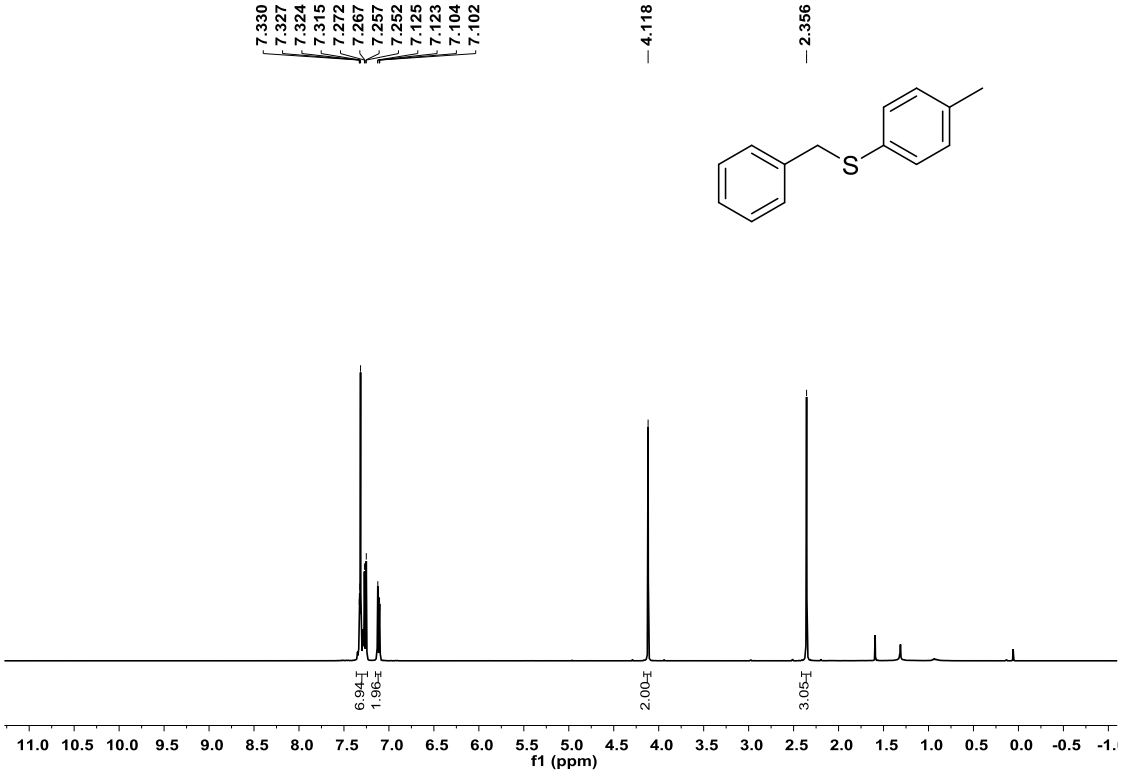
1-((4-methoxyphenyl)thio)propan-2-one (5bf)[6]: light yellow liquid was obtained with 33% yield. Eluent: Petroleum ether: CH_2Cl_2 = 4:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.35 (d, *J*=8.8, 2H), 6.85 (d, *J*=8.8, 2H), 3.79 (s, 3H), 3.56 (s, 2H), 2.26 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 203.7, 159.5, 133.6, 124.5, 114.8, 55.3, 46.5, 28.1.



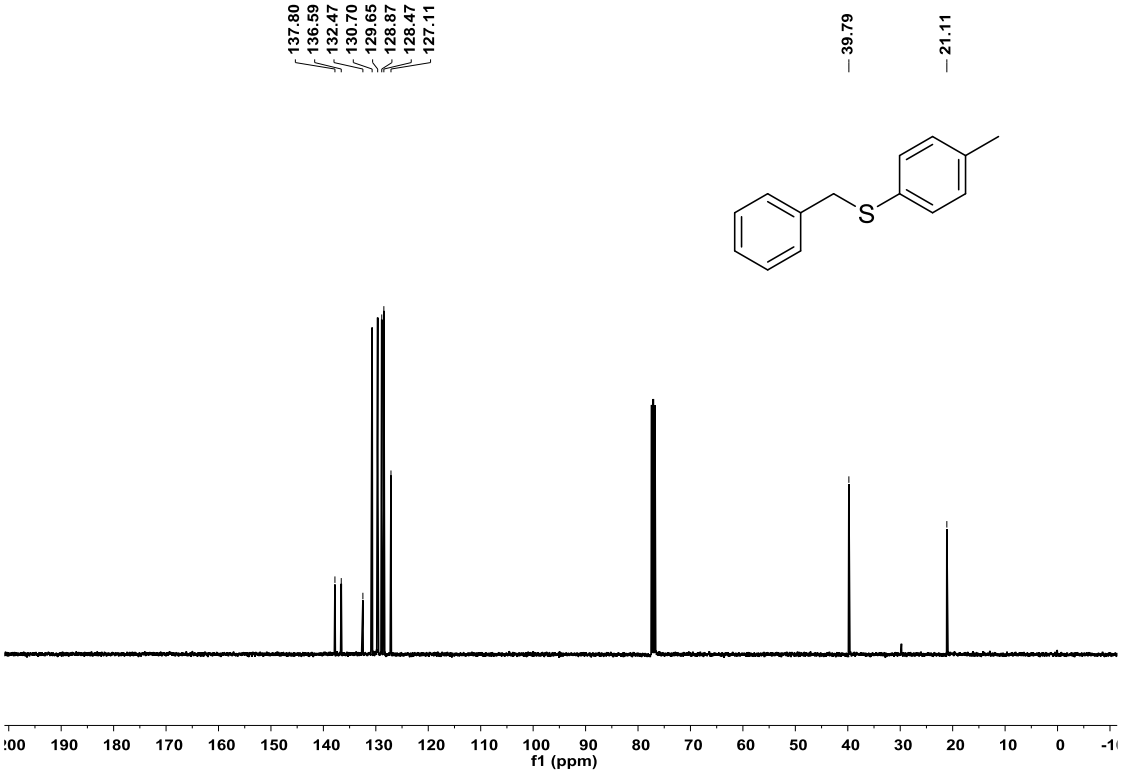
4-hydroxy-3-((4-methoxyphenyl)thio)pent-3-en-2-one (5cf)[7]: colorless crystal was obtained with 90% yield. Eluent: Petroleum ether: CH_2Cl_2 = 4:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 17.22 (s, 1H), 7.07 (d, *J*=8.8, 2H), 6.87 (d, *J*=8.8, 2H), 3.81 (s, 3H), 2.38 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 198.1, 157.9, 128.4, 126.9, 115.0, 103.1, 55.4, 24.5.

Copies of NMR spectrums

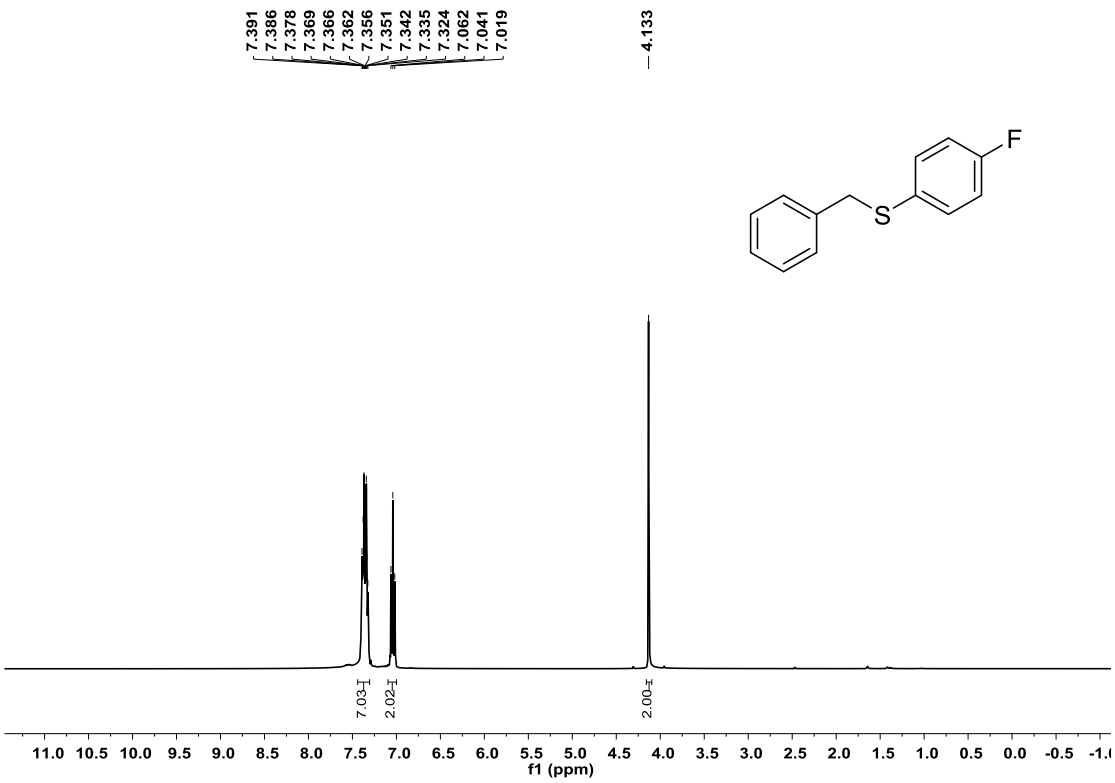
^{1}H NMR of **benzyl phenyl sulfide** (**3aa**)



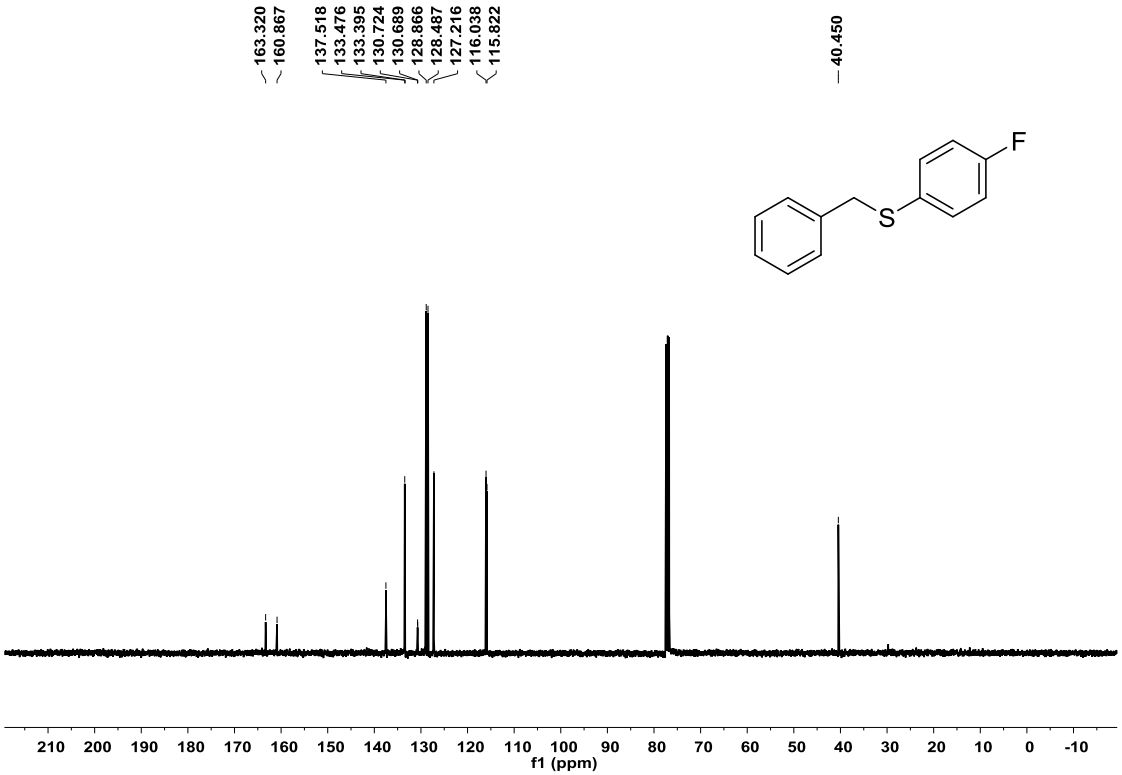
^{13}C NMR of **benzyl phenyl sulfide** (**3aa**)



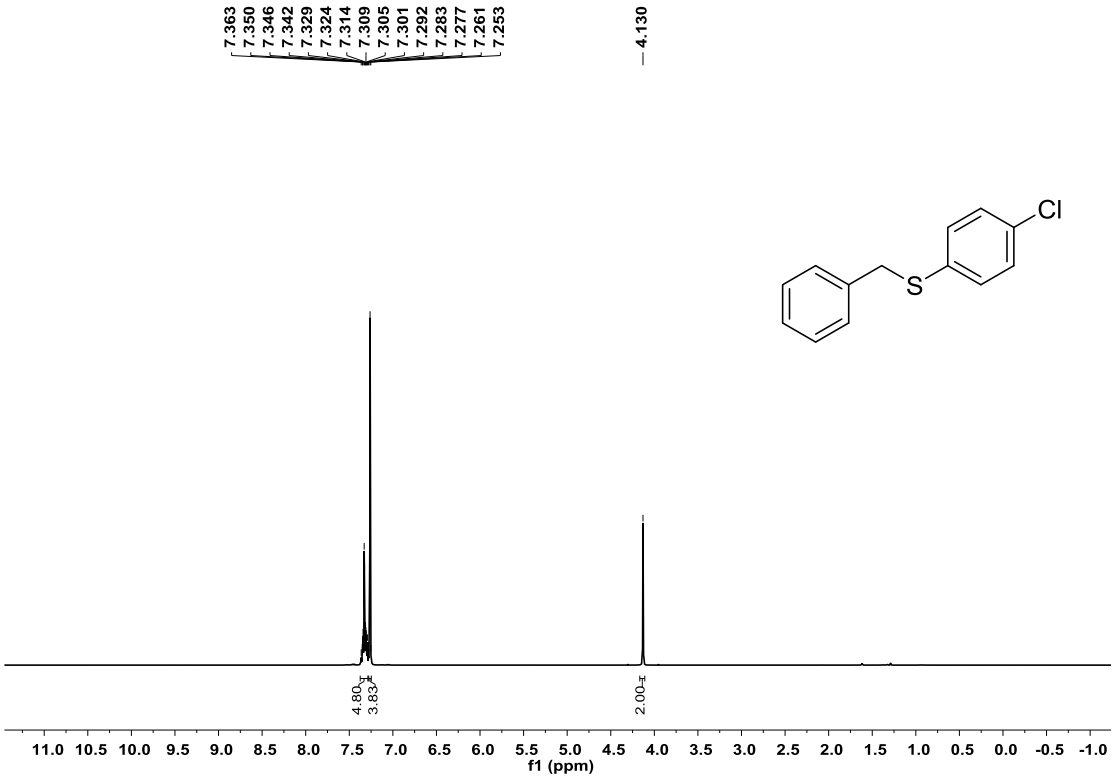
^{1}H NMR of **benzyl 4-fluorophenyl sulfide** (**3ab**)



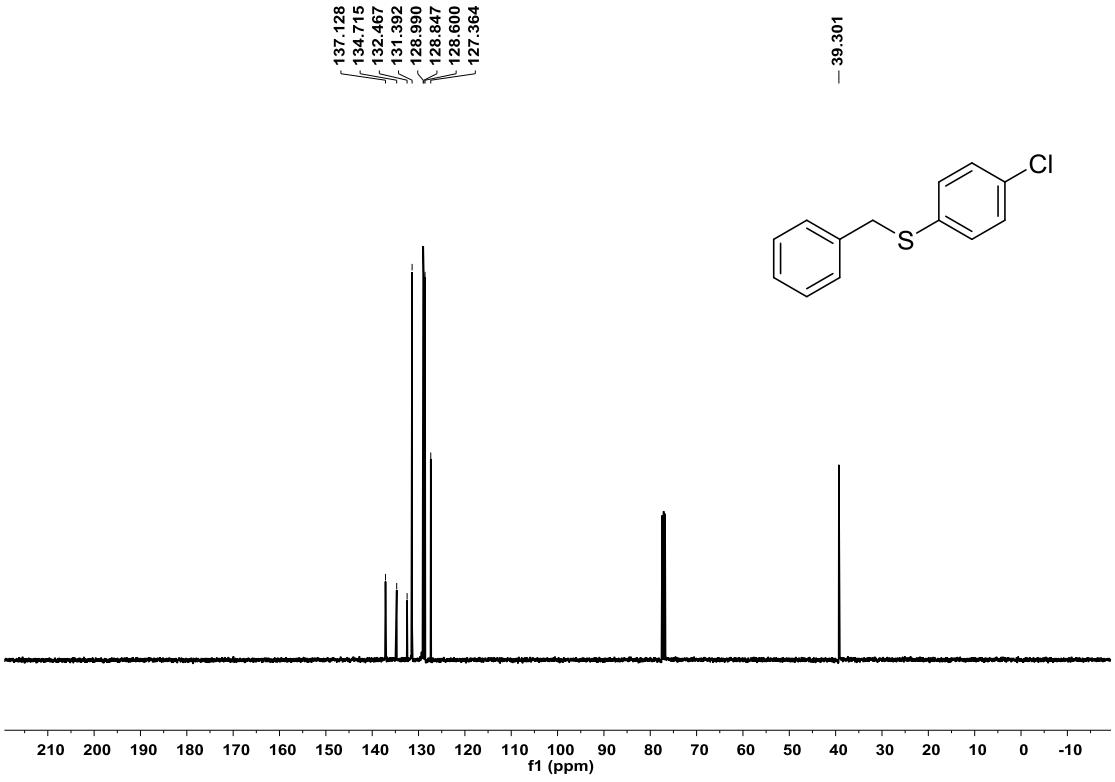
^{13}C NMR of **benzyl 4-fluorophenyl sulfide** (**3ab**)



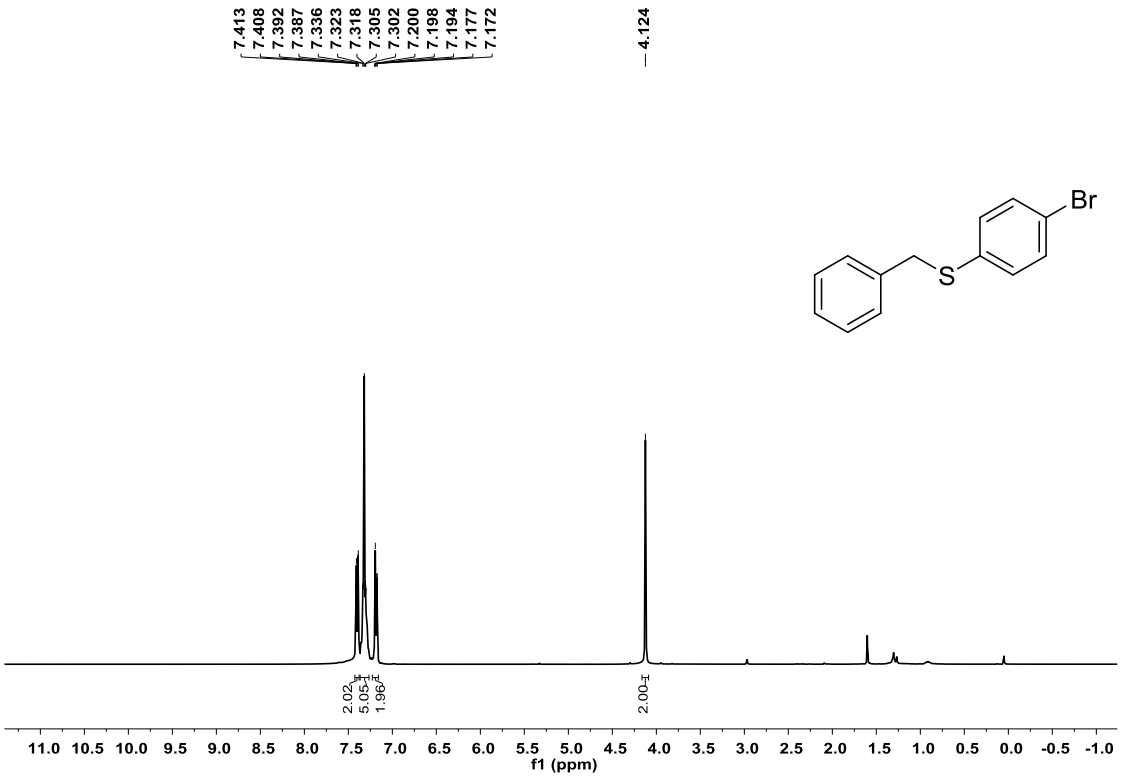
^{1}H NMR of **benzyl 4-chlorophenyl sulfide** (**3ac**)



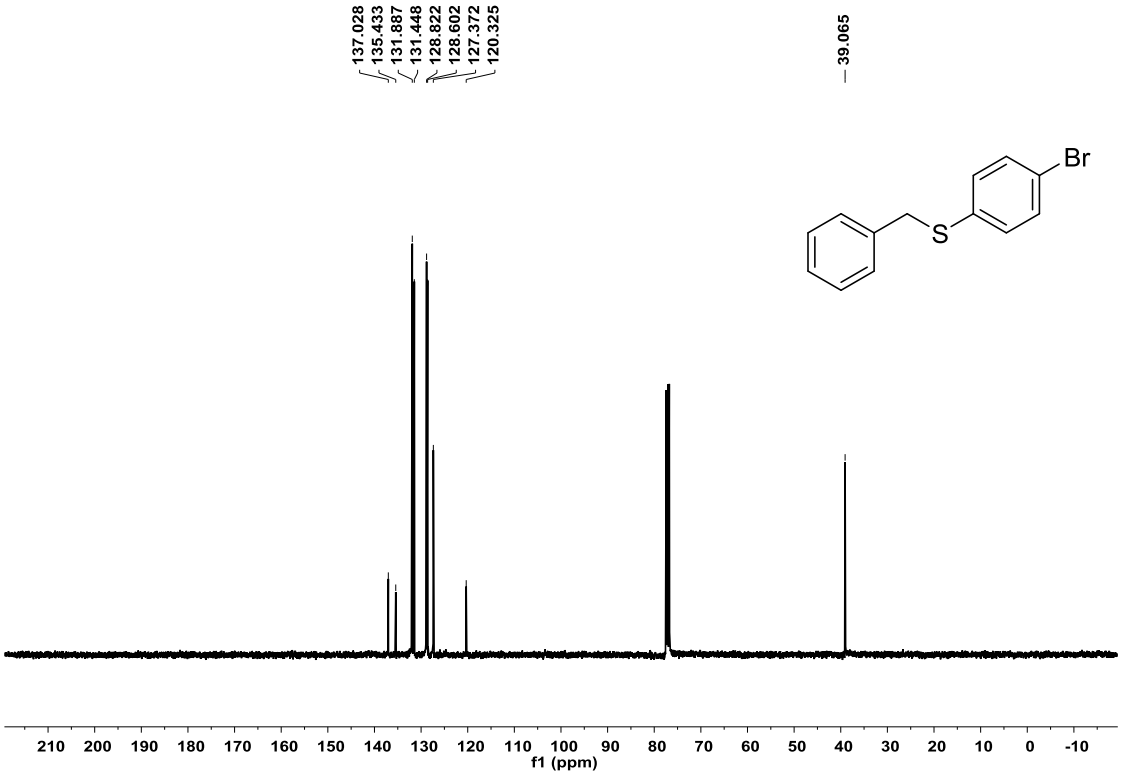
^{13}C NMR of **benzyl 4-chlorophenyl sulfide** (**3ac**)



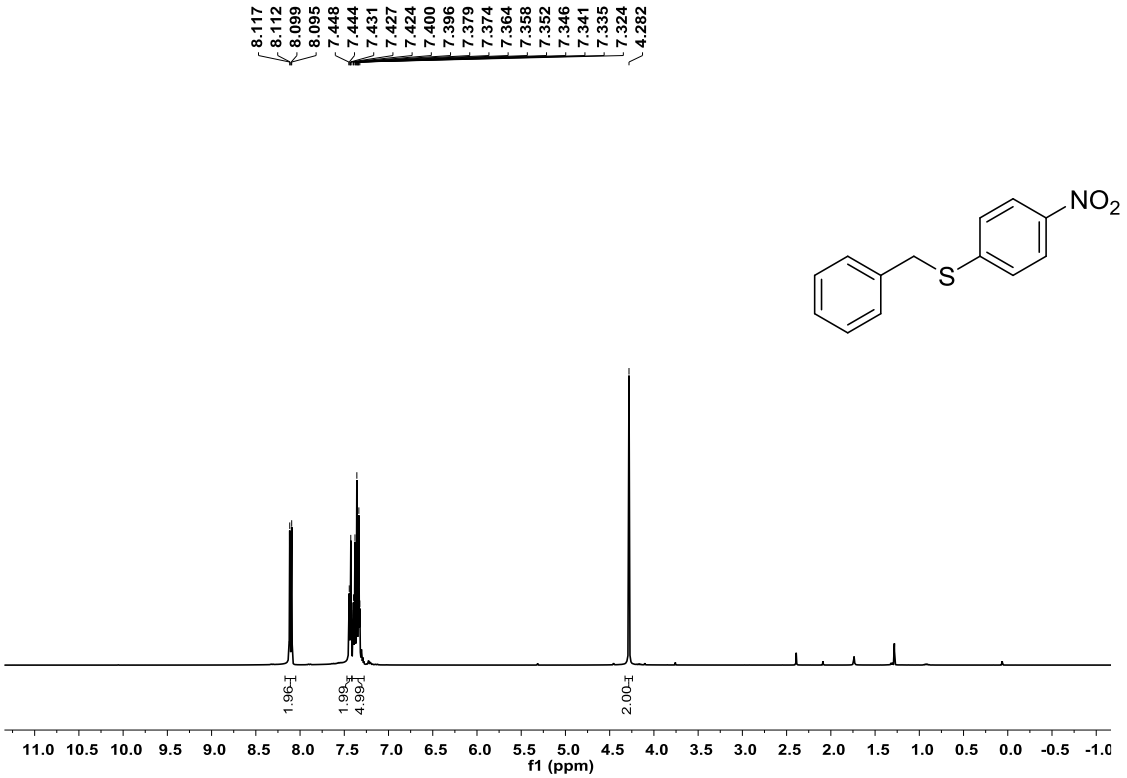
^{1}H NMR of **benzyl 4-bromophenyl sulfide** (**3ad**)



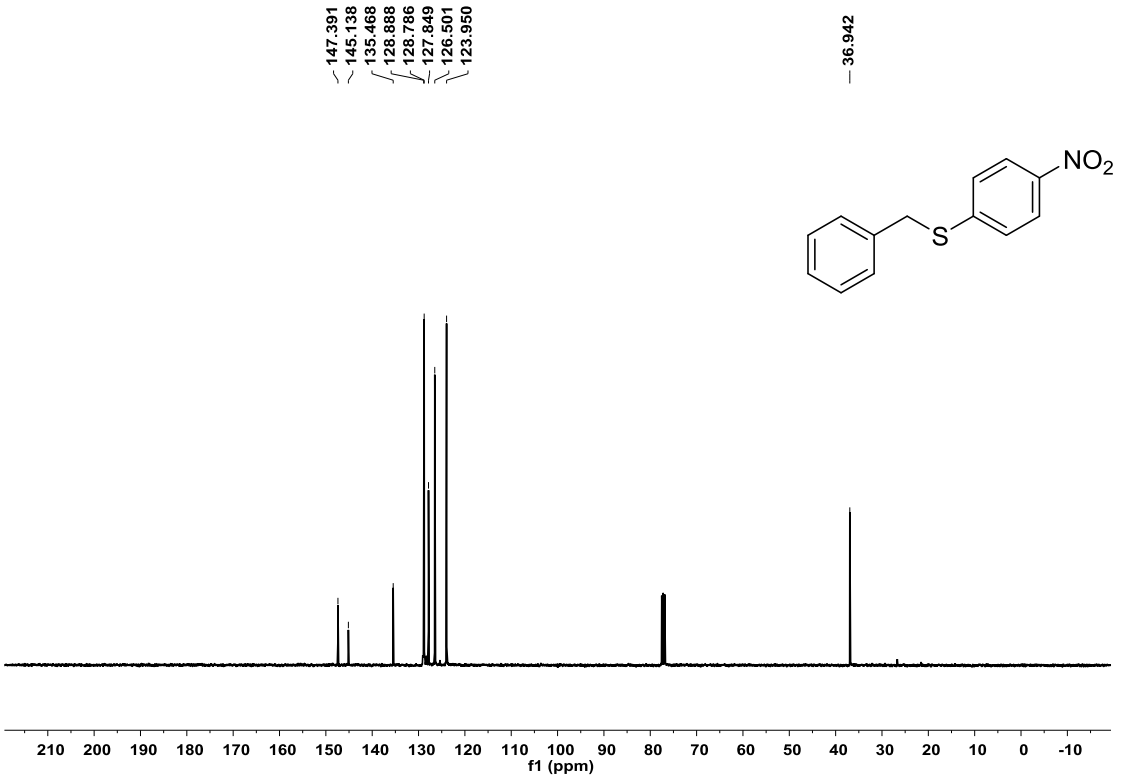
^{13}C NMR of **benzyl 4-bromophenyl sulfide** (**3ad**)



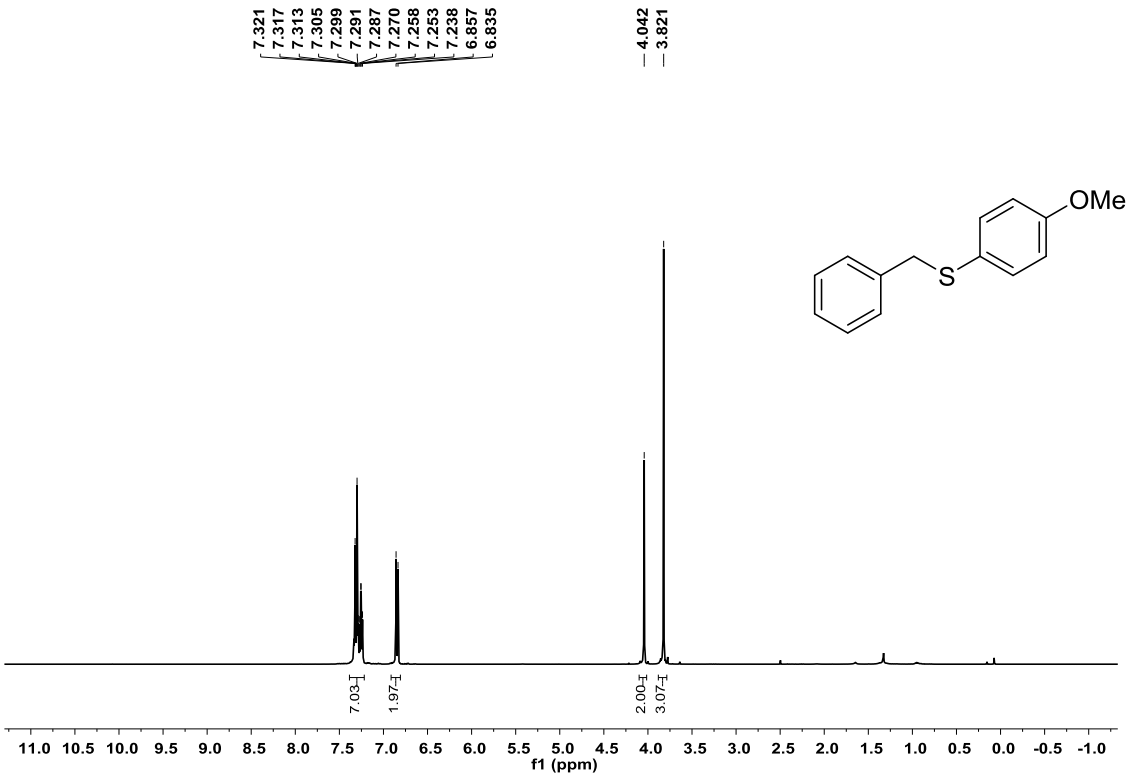
^{1}H NMR of **benzyl 4-nitrophenyl sulfide** (**3ae**)



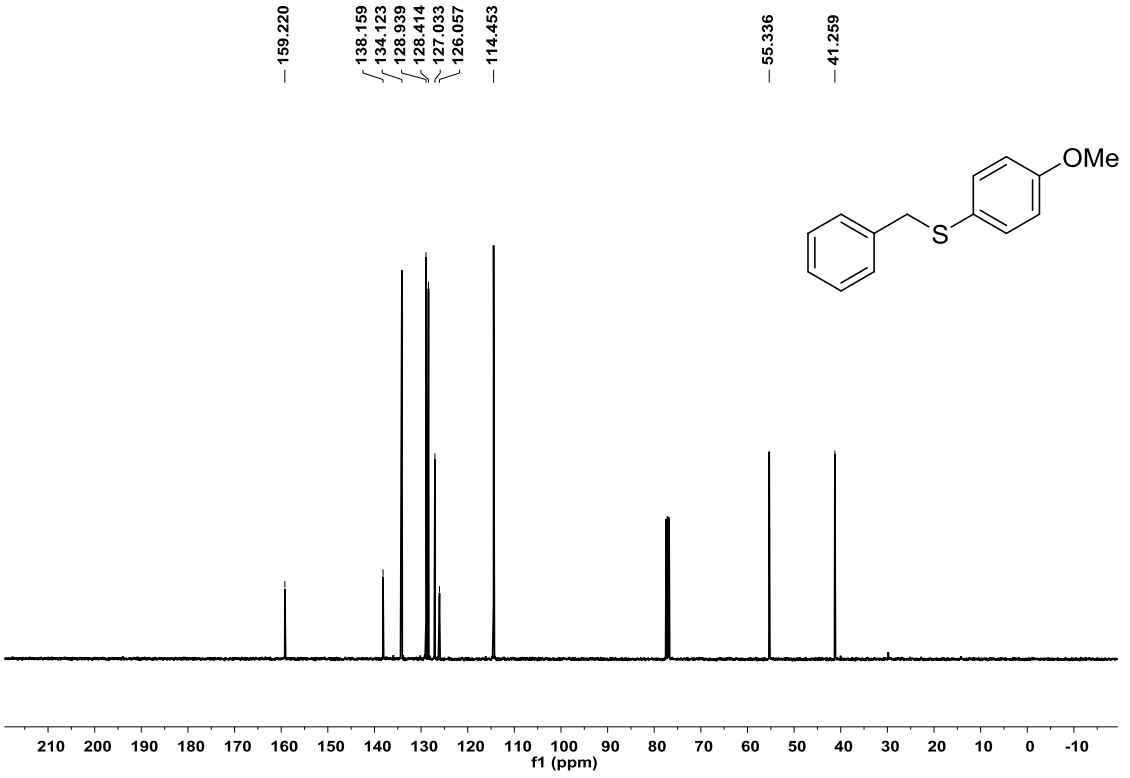
^{13}C NMR of **benzyl 4-nitrophenyl sulfide** (**3ae**)



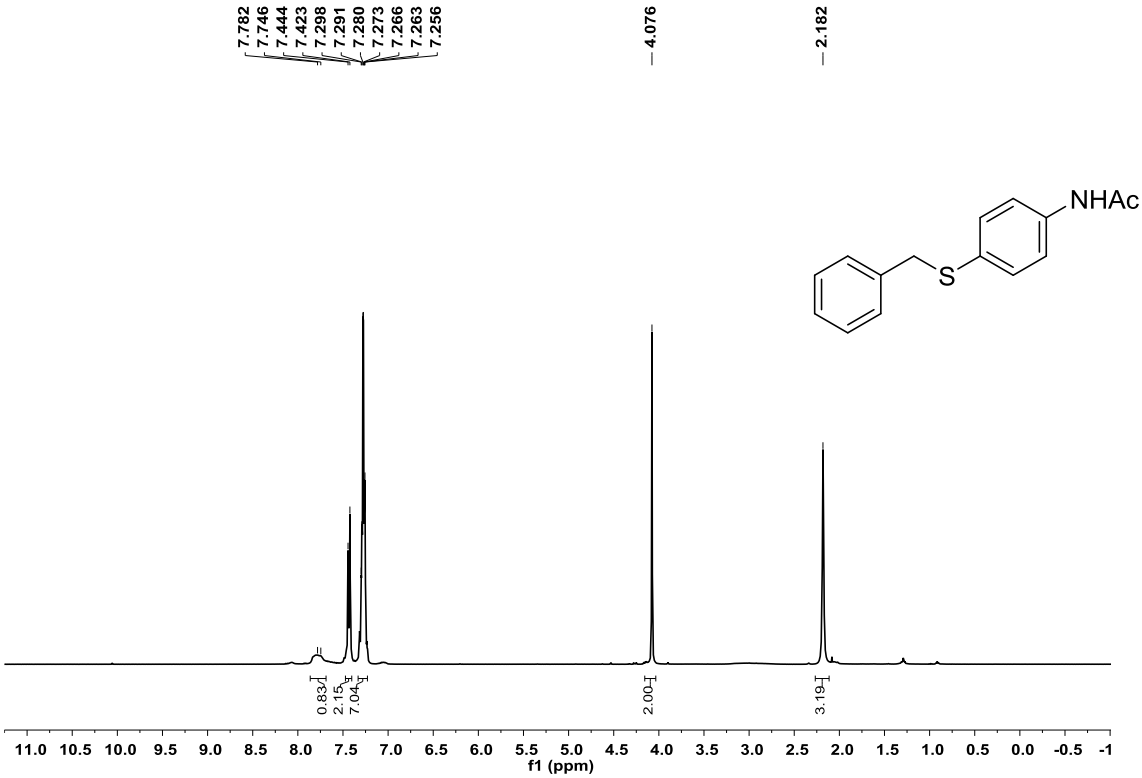
^{1}H NMR of **benzyl 4-nitrophenyl sulfide** (**3af**)



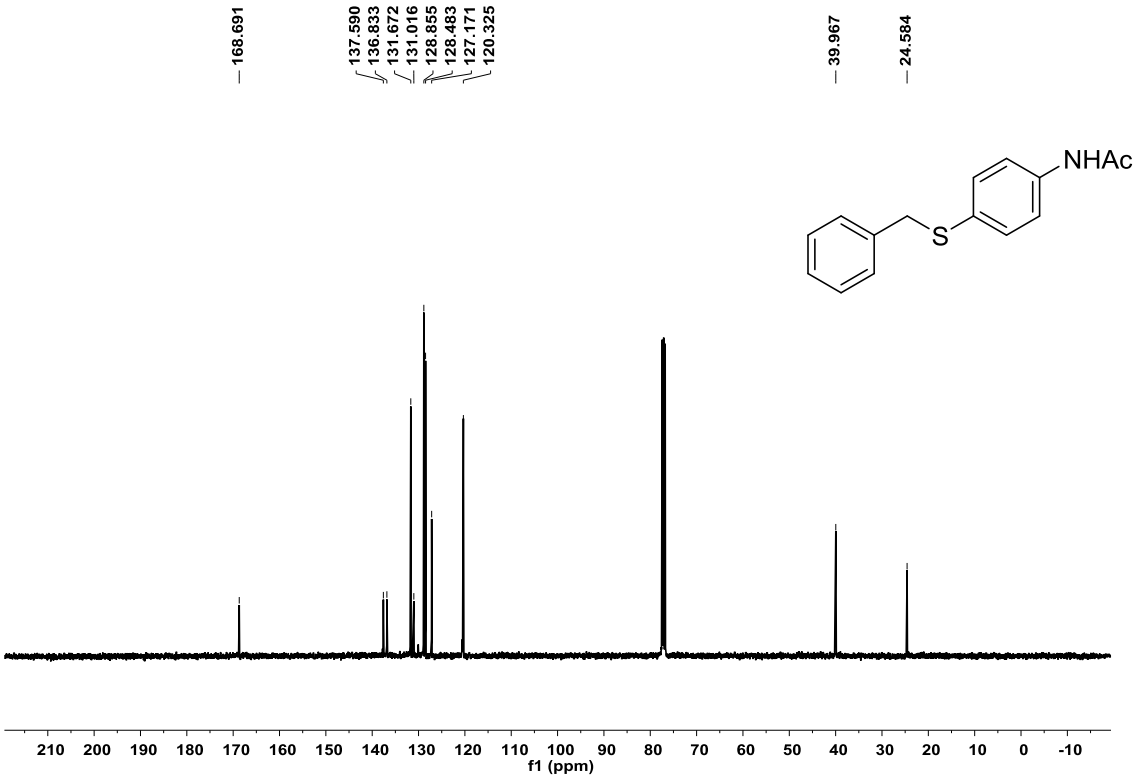
^{13}C NMR of **benzyl 4-nitrophenyl sulfide** (**3af**)



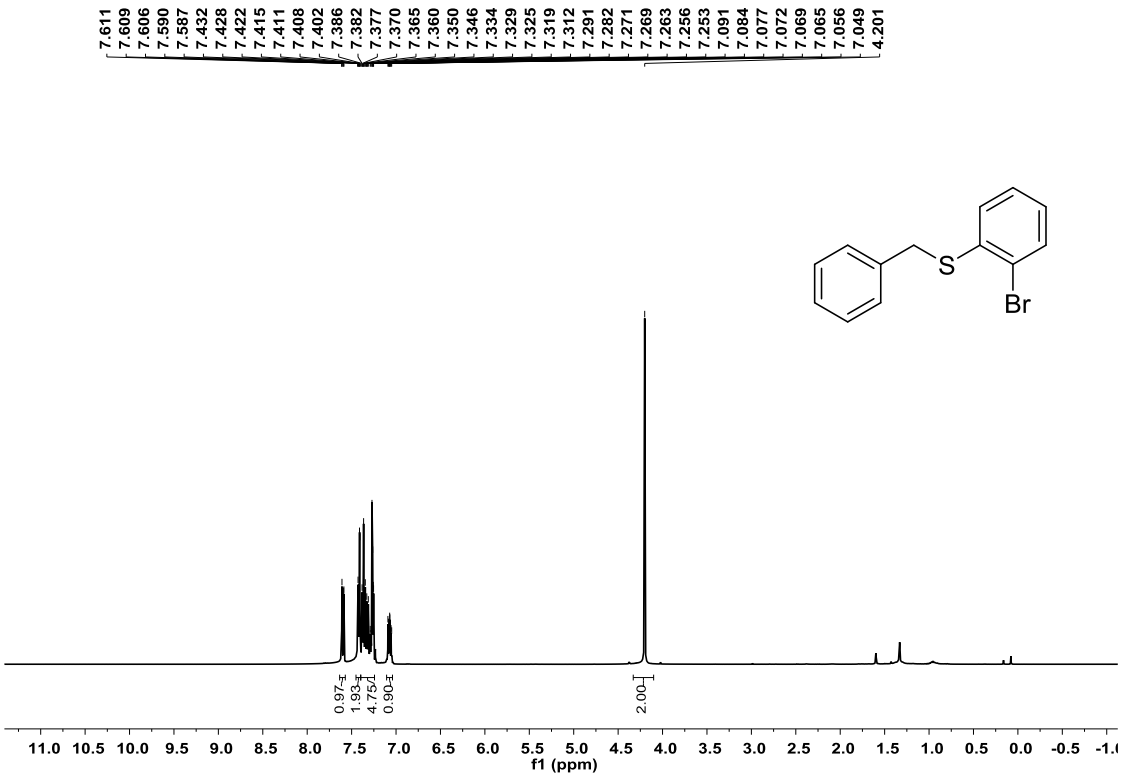
^{1}H NMR of **benzyl 4-nitrophenyl sulfide** (**3ag**)



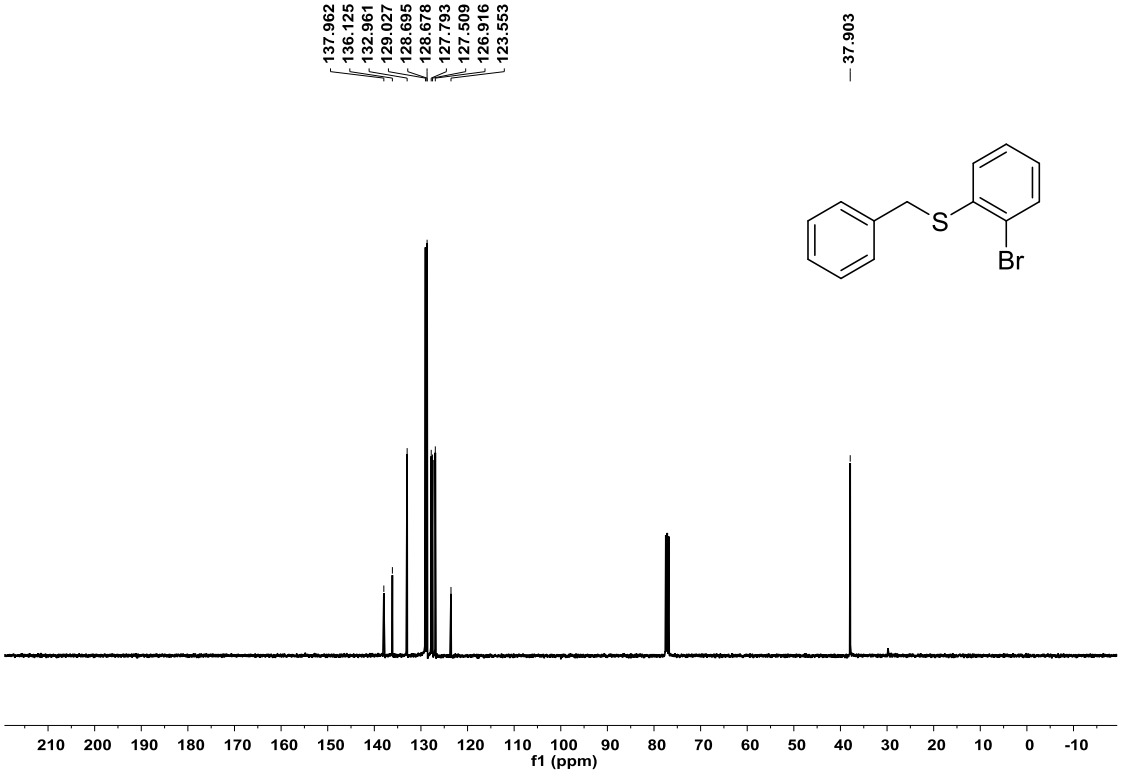
^{13}C NMR of **benzyl 4-nitrophenyl sulfide** (**3ag**)



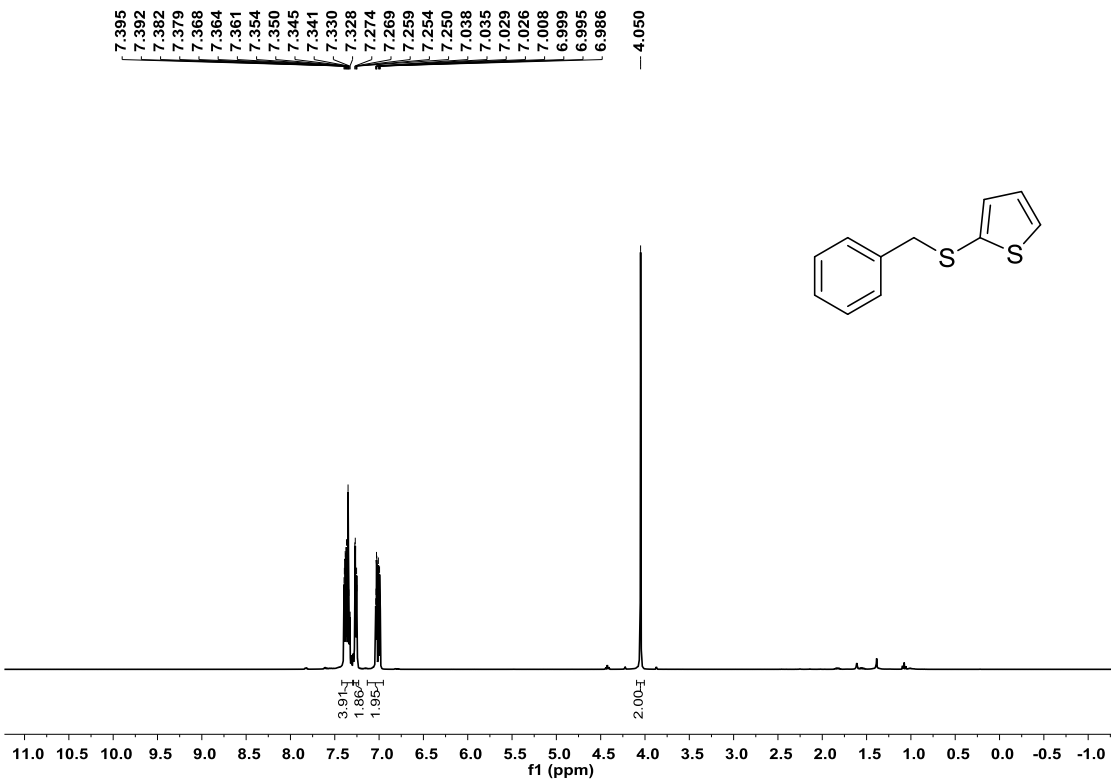
^{1}H NMR of **benzyl 2-bromophenyl sulfide** (**3ah**)



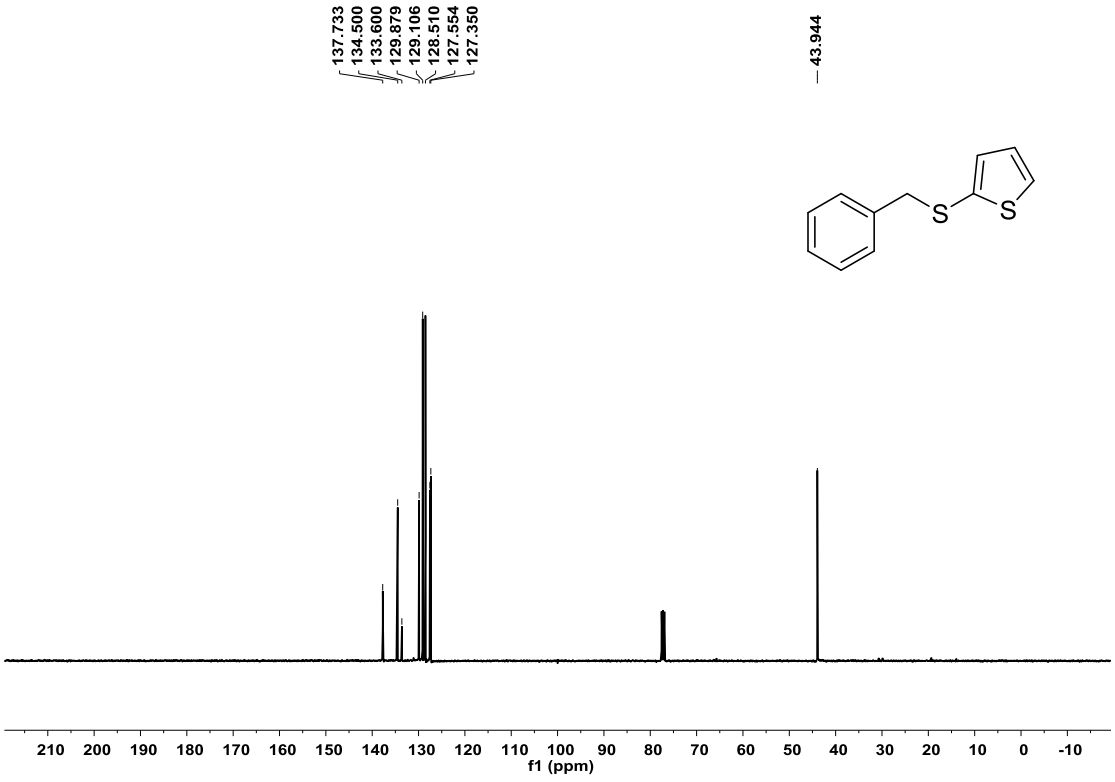
^{13}C NMR of **benzyl 2-bromophenyl sulfide** (**3ah**)



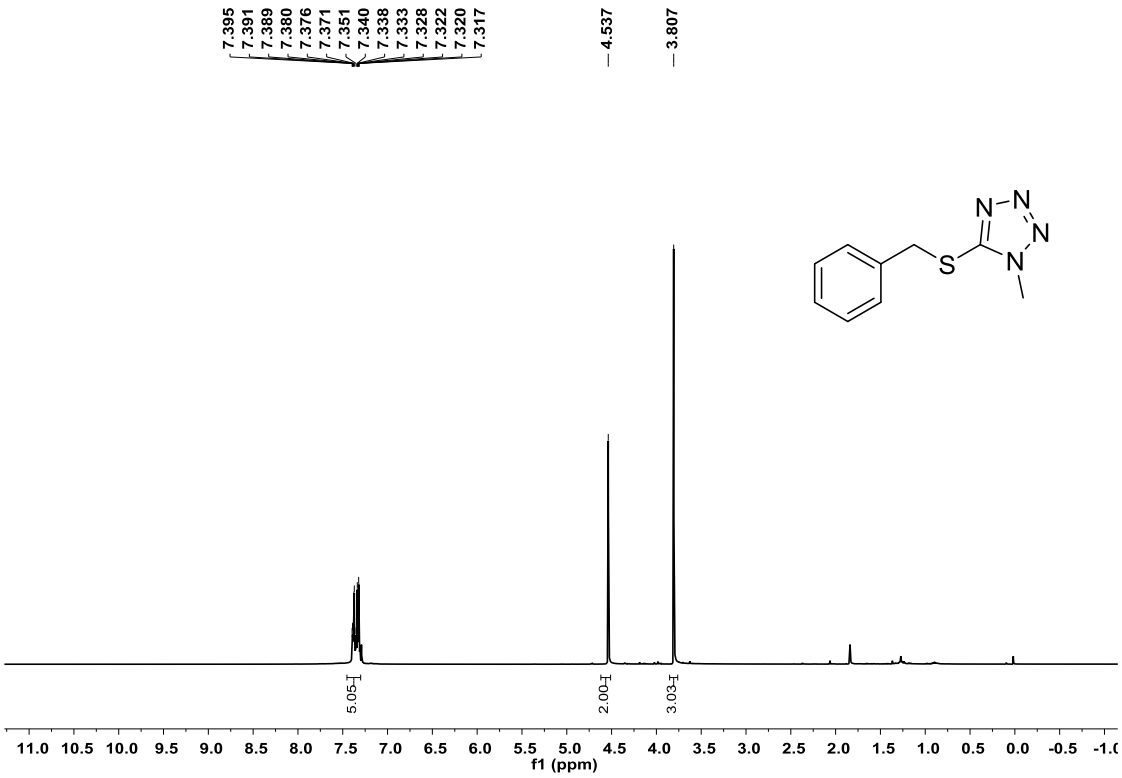
^{1}H NMR of **benzyl 2-thienyl sulfide** (**3ai**)



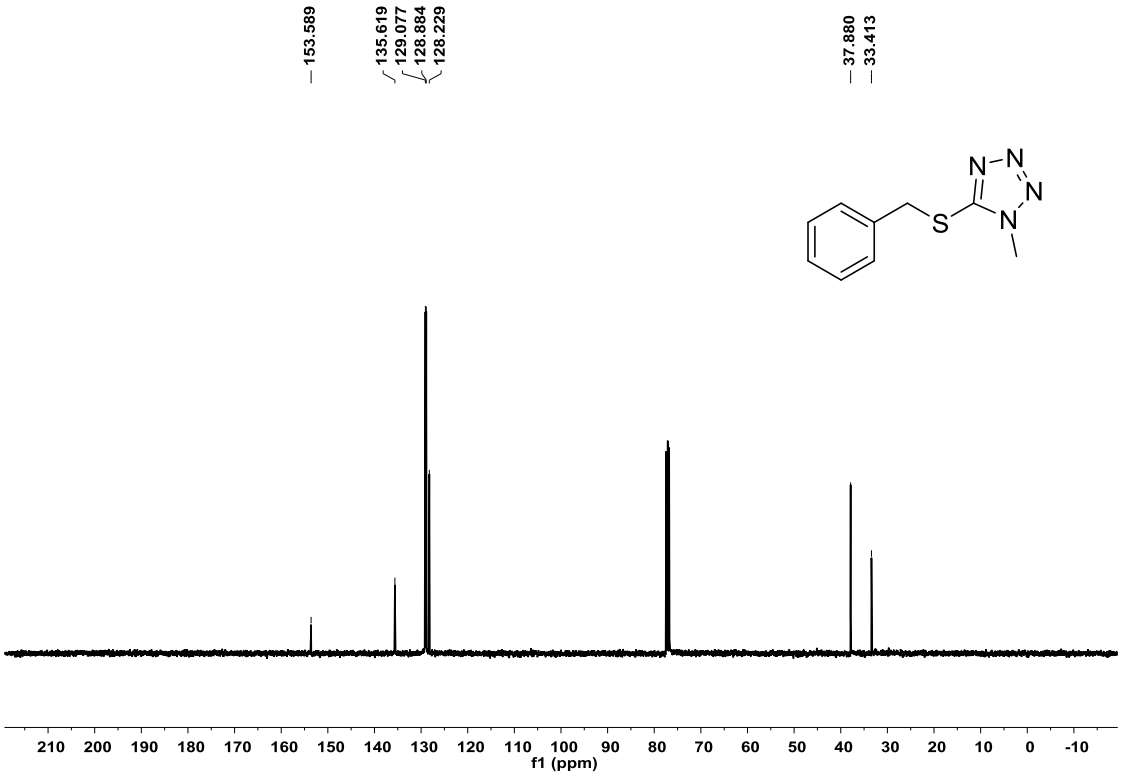
^{13}C NMR of **benzyl 2-thienyl sulfide** (**3ai**)



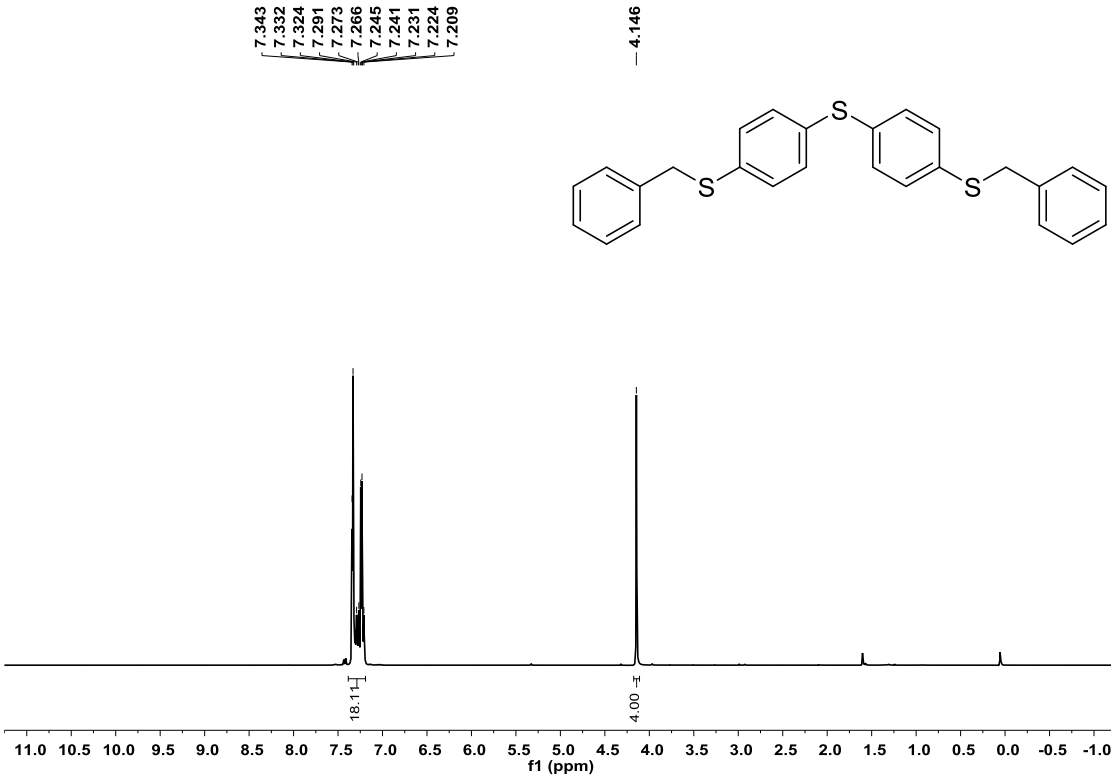
^{1}H NMR of **5-(benzylthio)-1-methyl-tetrazole** (**3aj**)



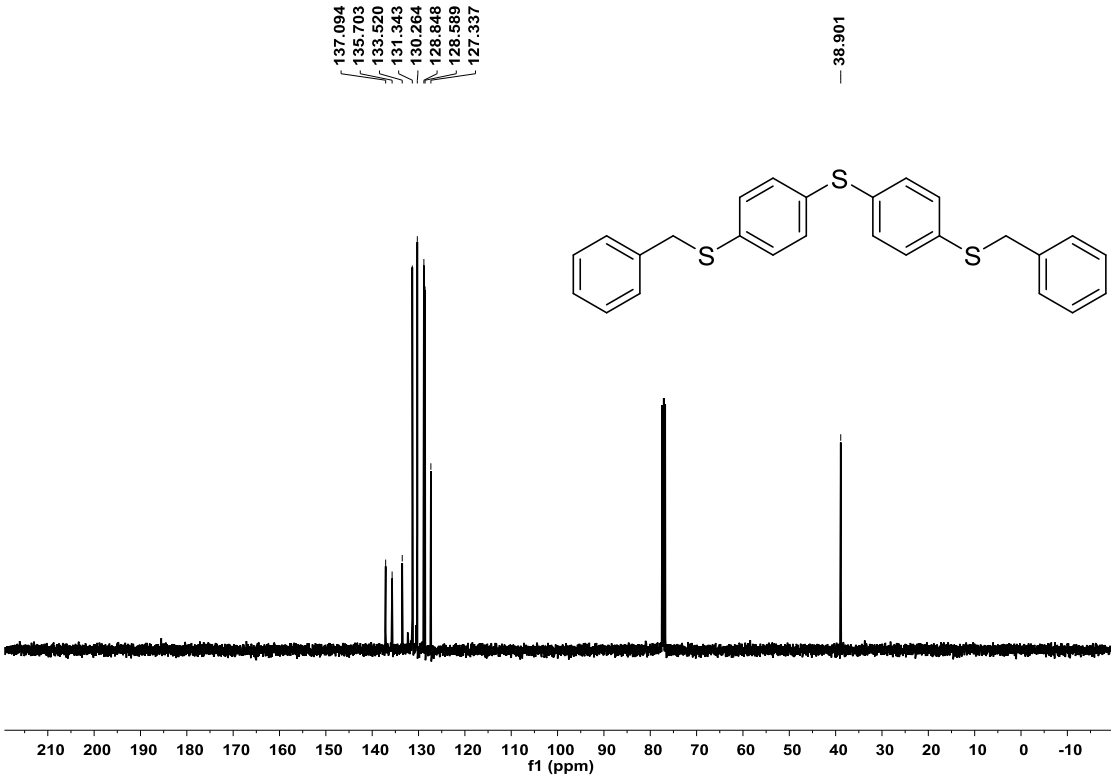
^{13}C NMR of **5-(benzylthio)-1-methyl-tetrazole** (**3aj**)



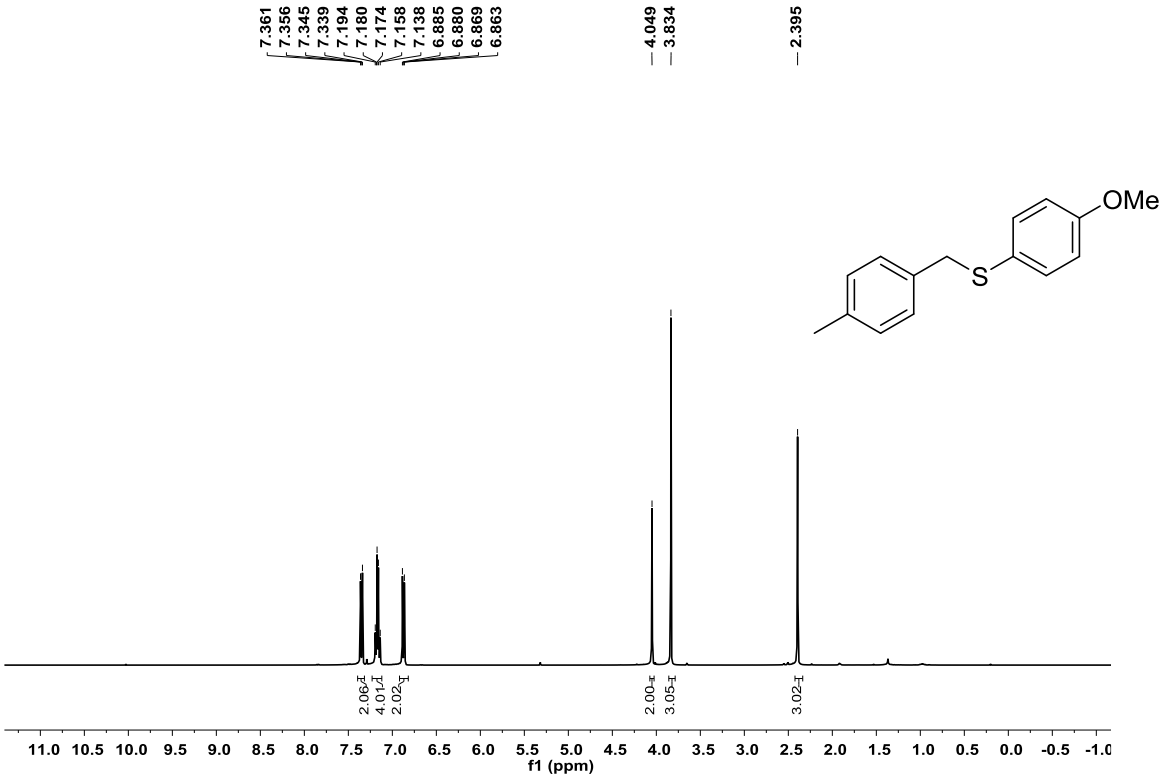
^{1}H NMR of **bis(4-(benzylthio)phenyl)sulfide** (**3ak**)



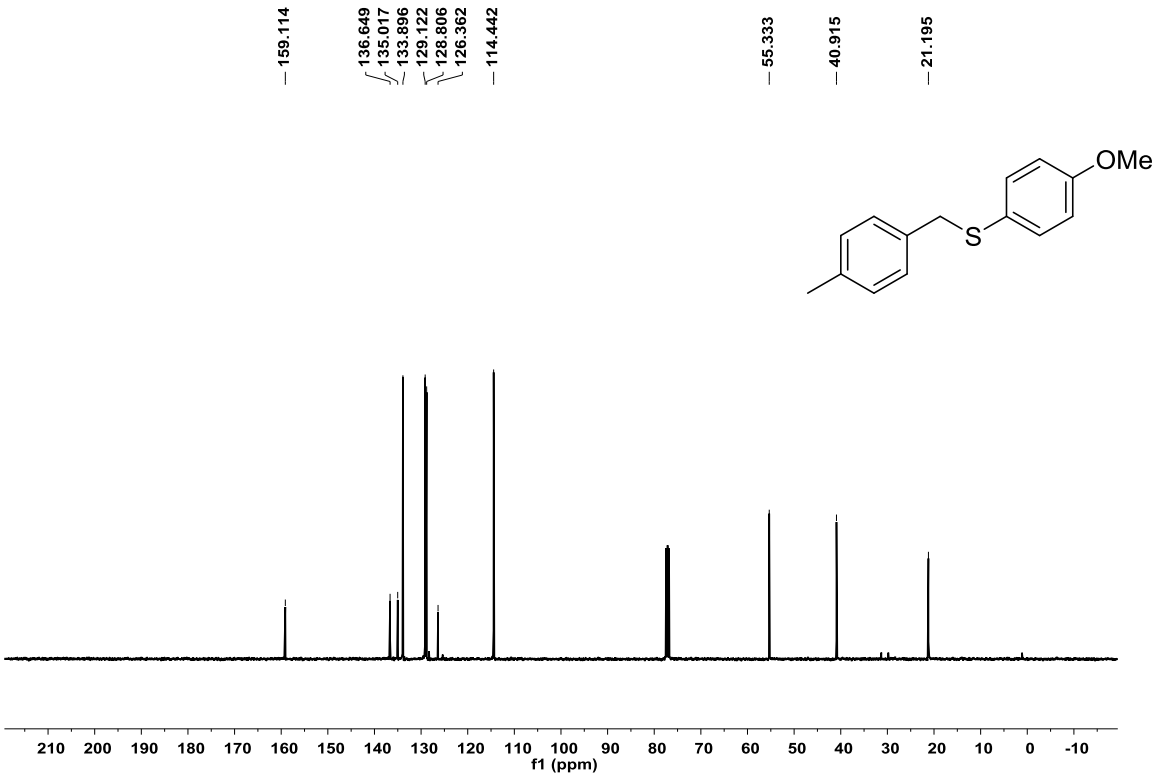
^{13}C NMR of **bis(4-(benzylthio)phenyl)sulfide** (**3ak**)



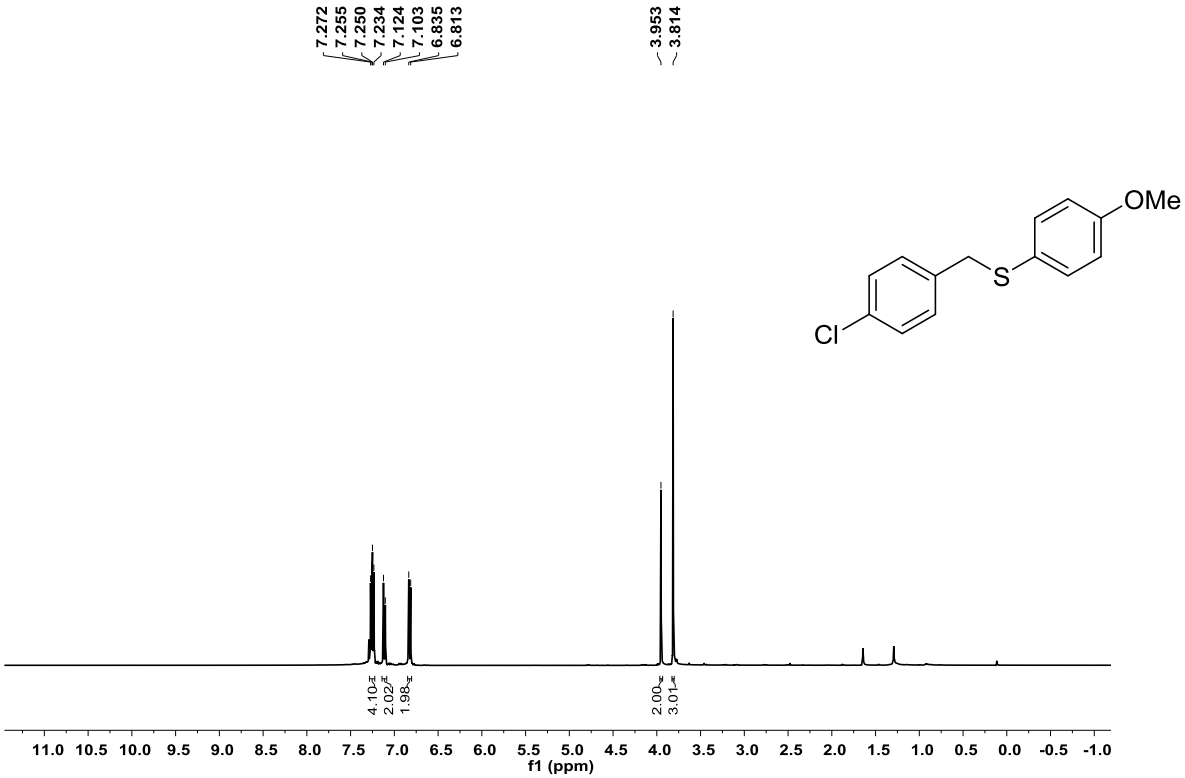
^{1}H NMR of **4-methylbenzyl 4-methoxyphenyl sulfide** (**3bf**)



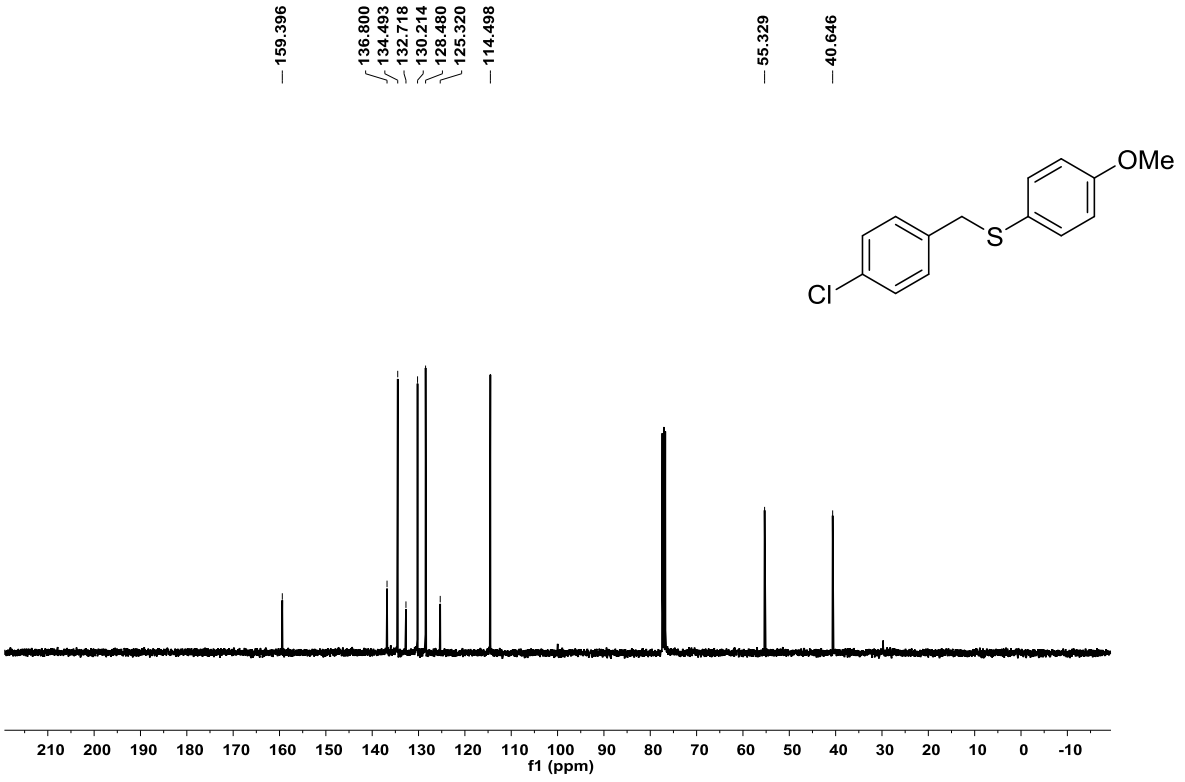
^{13}C NMR of **4-methylbenzyl 4-methoxyphenyl sulfide** (**3bf**)



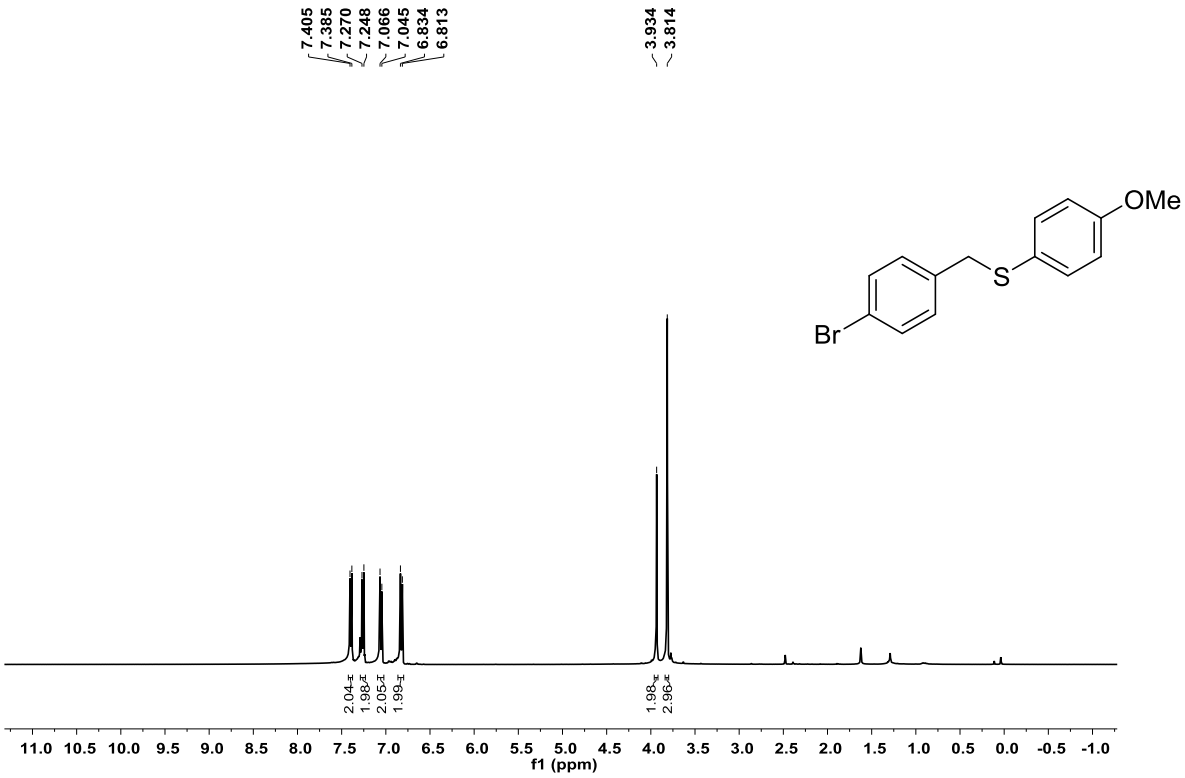
^{1}H NMR of **4-chlorobenzyl 4-methoxyphenyl sulfide** (**3cf**)



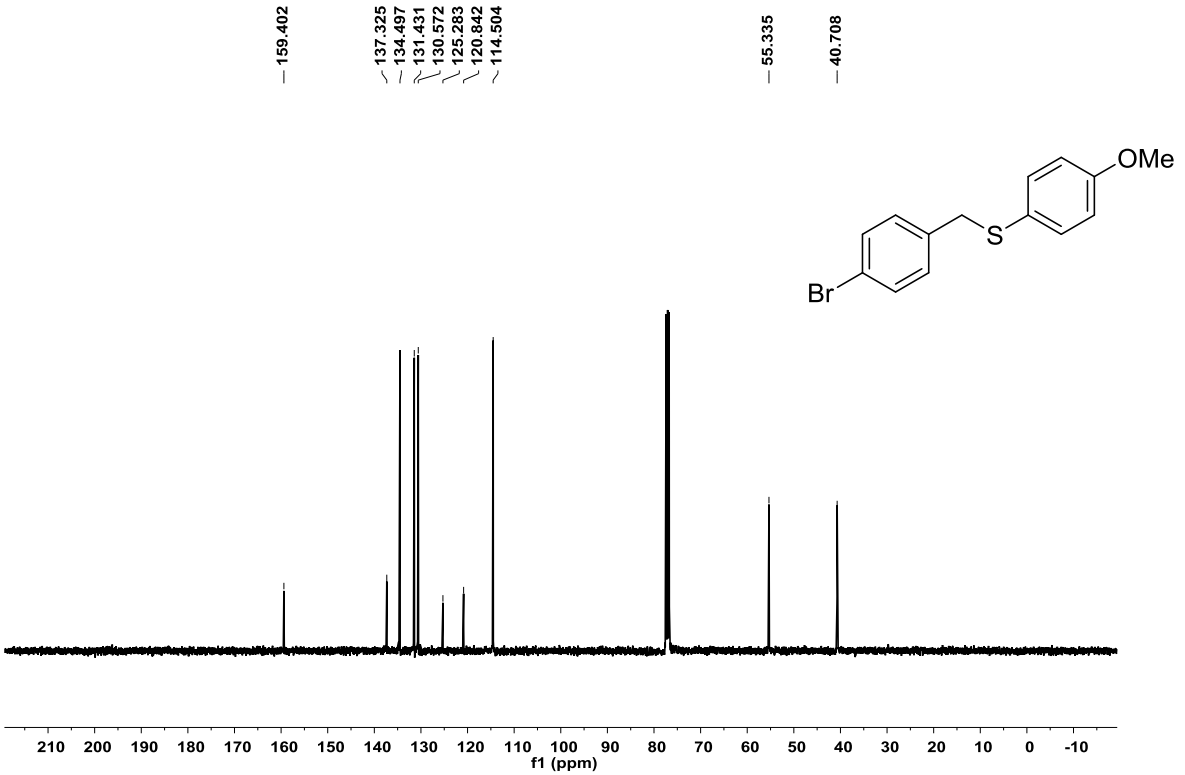
^{13}C NMR of **4-chlorobenzyl 4-methoxyphenyl sulfide** (**3cf**)



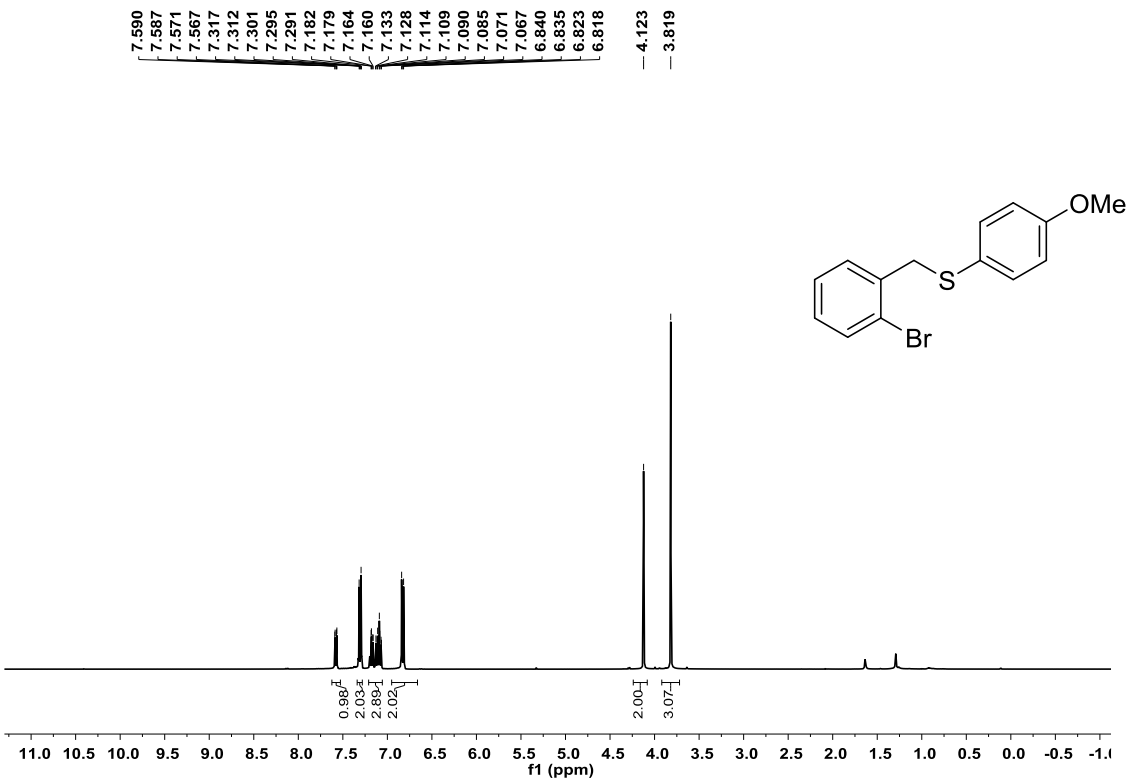
^{1}H NMR of **4-bromobenzyl 4-methoxyphenyl sulfide** (**3df**)



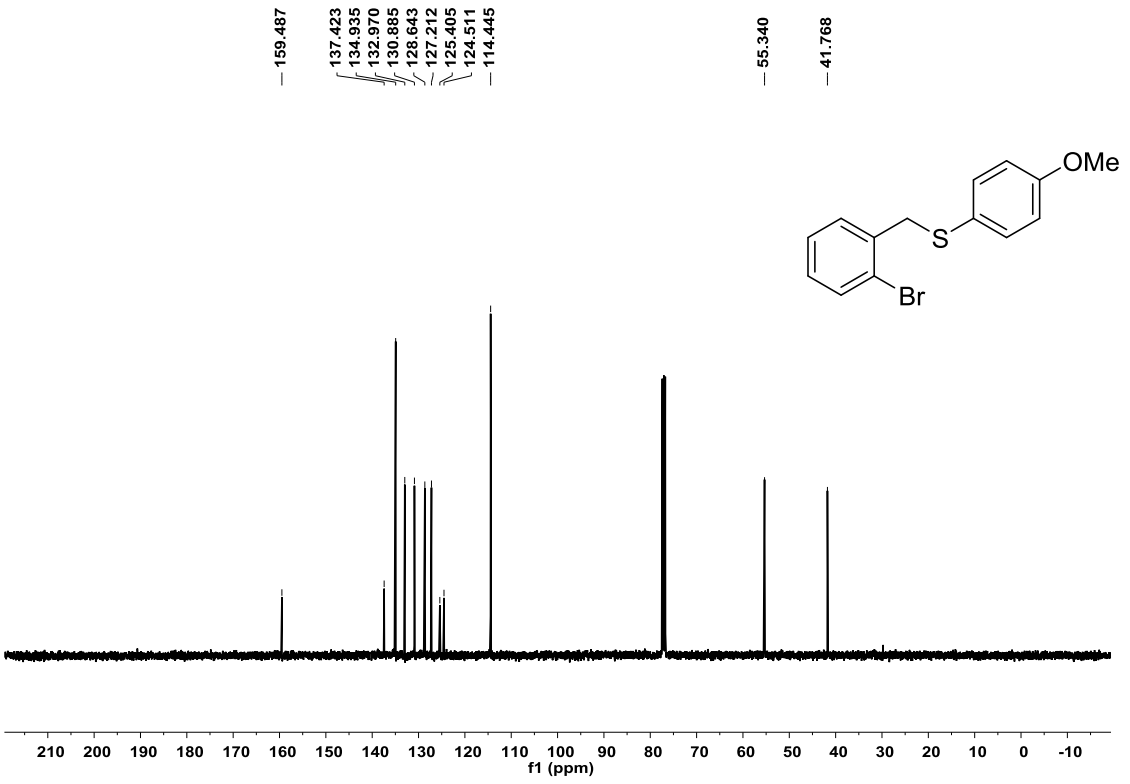
^{13}C NMR of **4-bromobenzyl 4-methoxyphenyl sulfide** (**3df**)



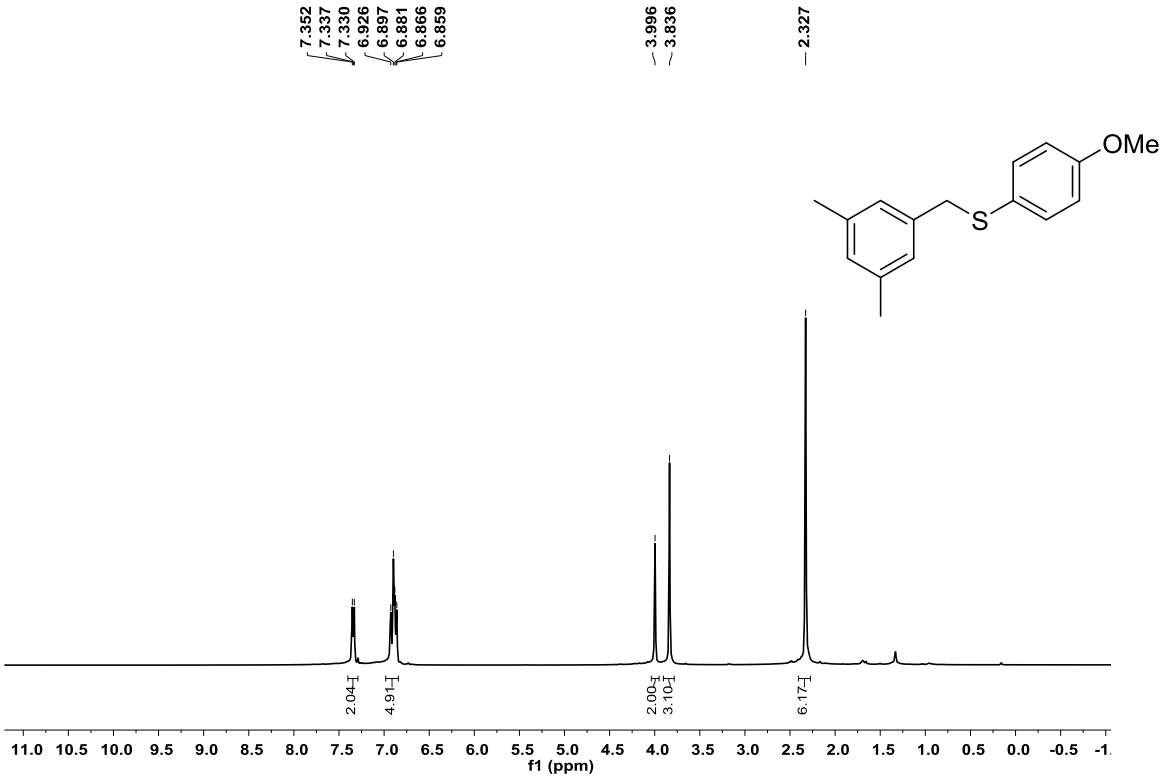
^{1}H NMR of **2-bromobenzyl 4-methoxyphenyl sulfide** (**3ef**)



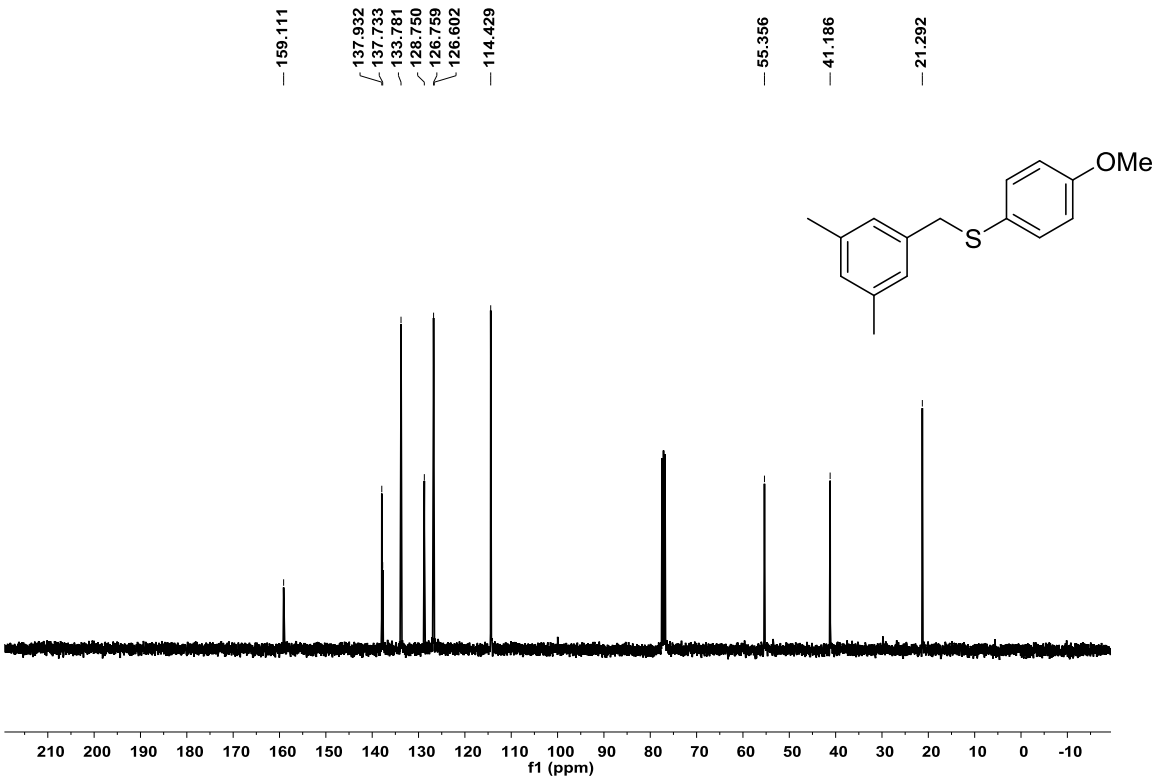
^{13}C NMR of **2-bromobenzyl 4-methoxyphenyl sulfide** (**3ef**)



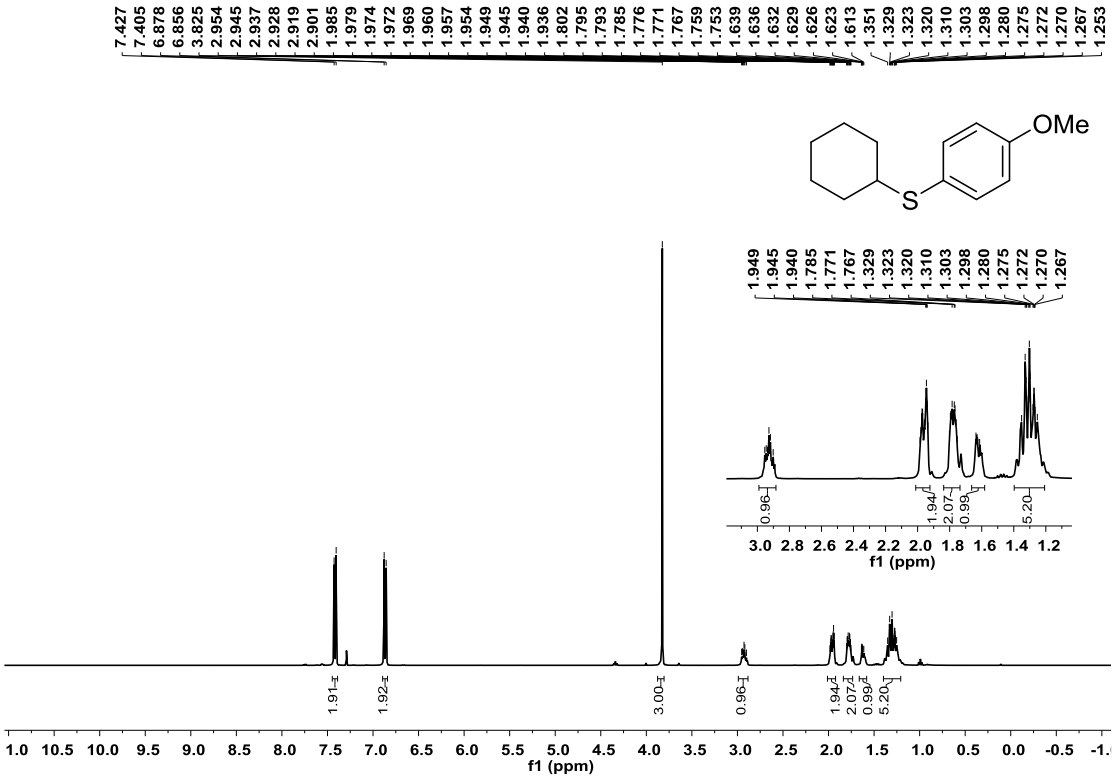
^{1}H NMR of **3-5-dimethylbenzyl 4-methoxyphenyl sulfide** (**3ff**)



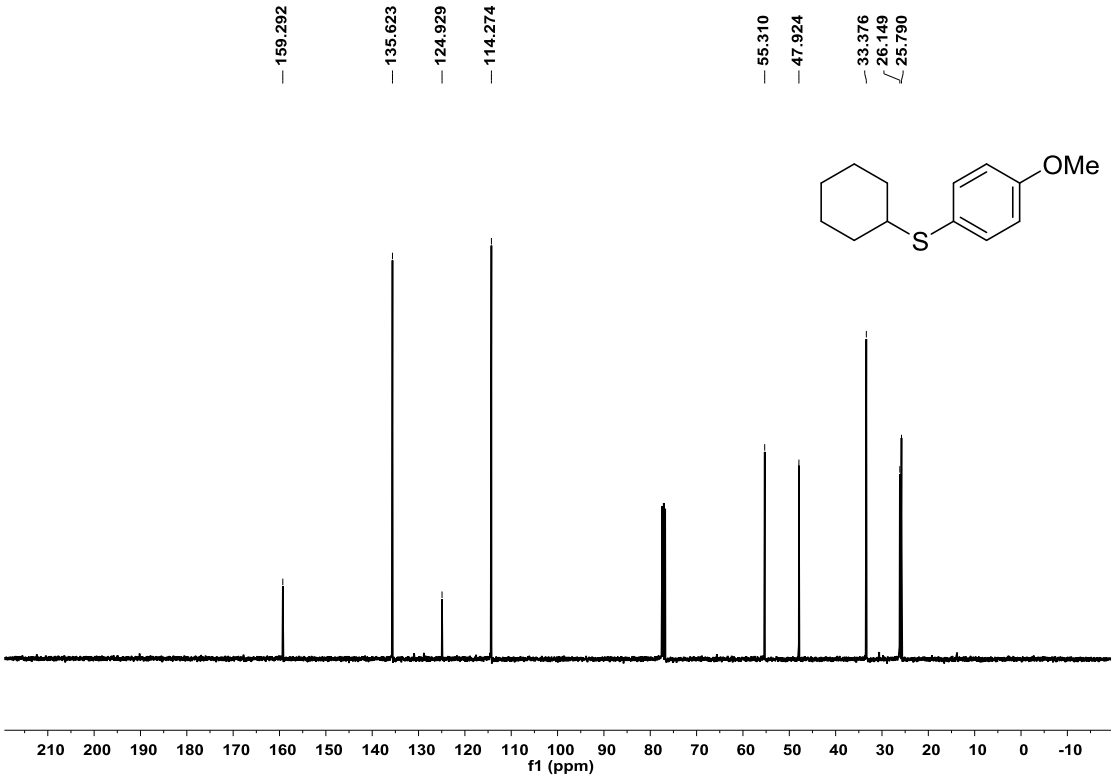
^{13}C NMR of **3-5-dimethylbenzyl 4-methoxyphenyl sulfide** (**3ff**)



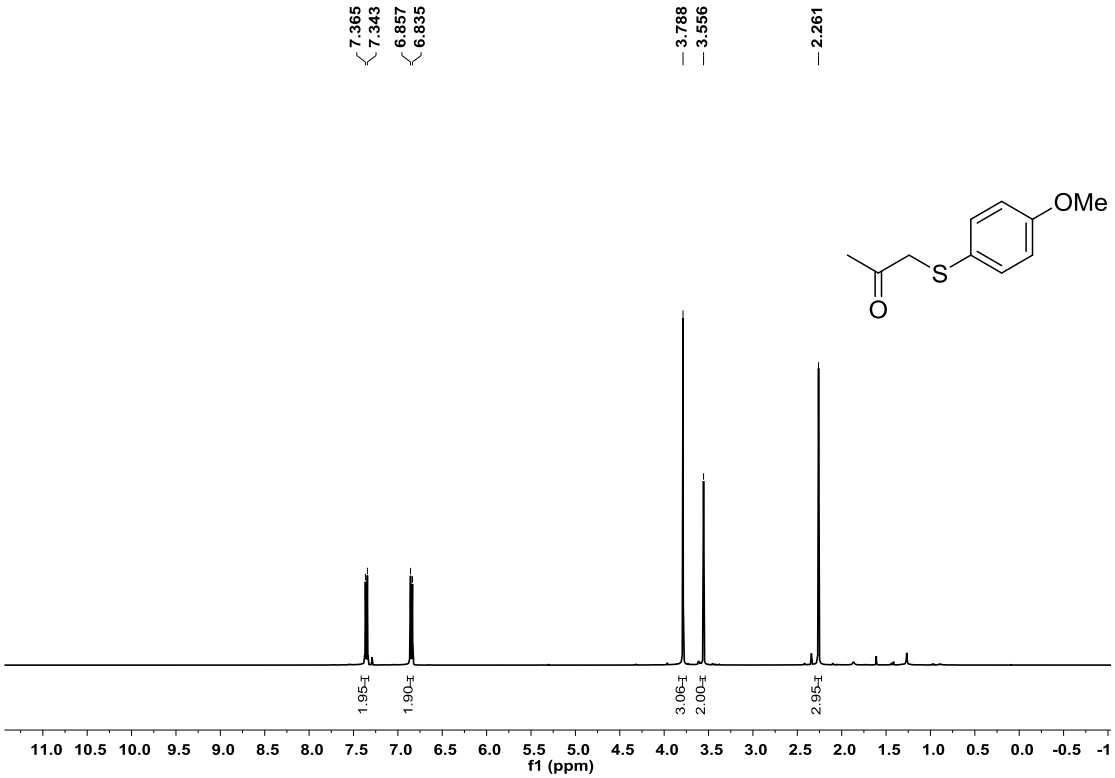
^{1}H NMR of **cyclohexyl 4-methoxyphenyl sulfide** (**5af**)



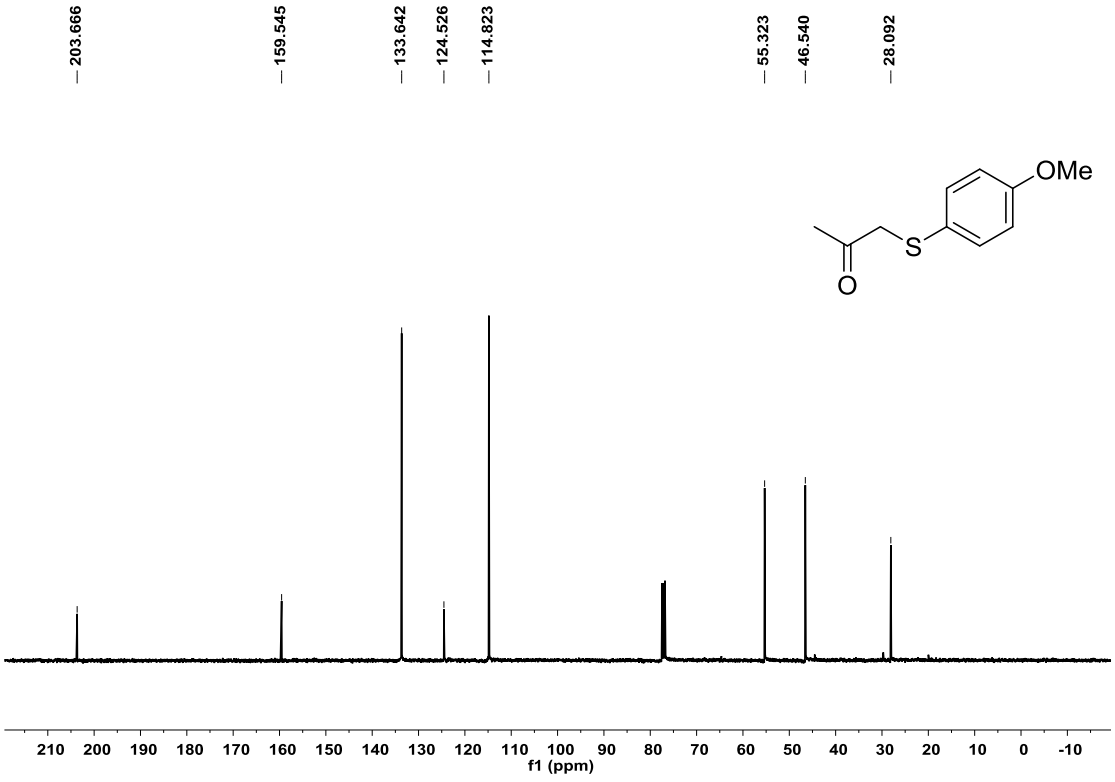
^{13}C NMR of **cyclohexyl 4-methoxyphenyl sulfide** (**5af**)



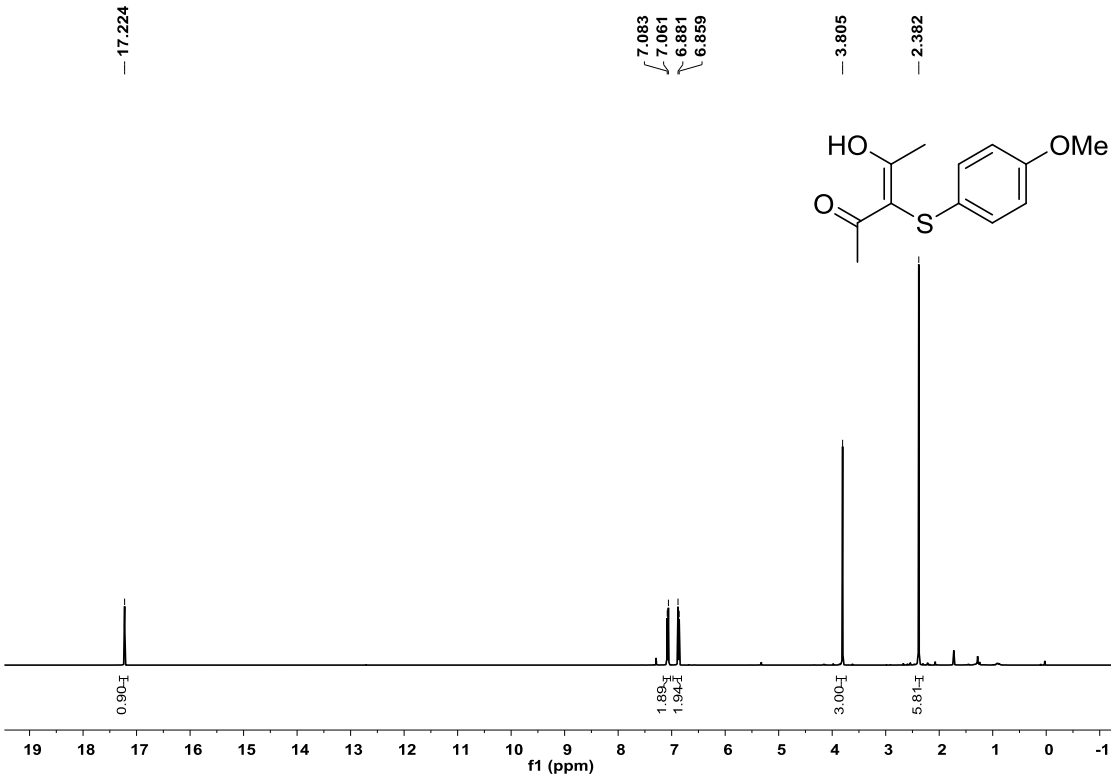
^{1}H NMR of **1-((4-methoxyphenyl)thio)propan-2-one** (**5bf**)



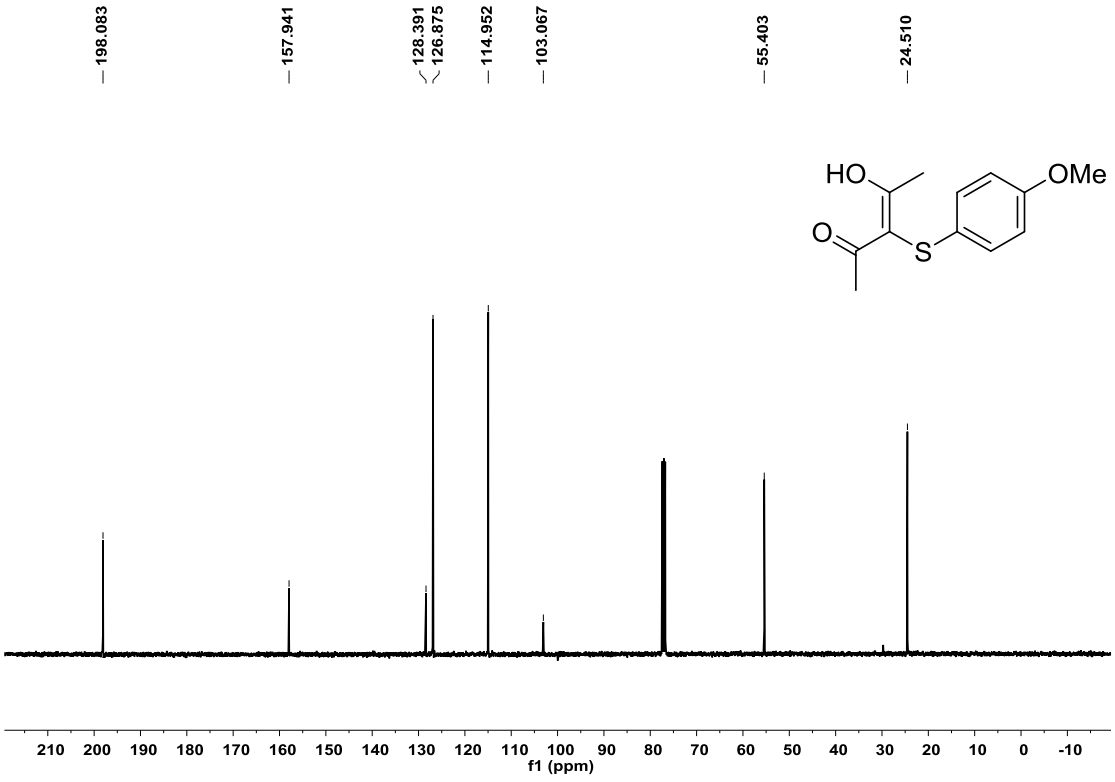
^{13}C NMR of **1-((4-methoxyphenyl)thio)propan-2-one** (**5bf**)



^{1}H NMR of **4-hydroxy-3-((4-methoxyphenyl)thio)pent-3-en-2-one** (**5cf**)



^{13}C NMR of **4-hydroxy-3-((4-methoxyphenyl)thio)pent-3-en-2-one** (**5cf**)



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